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PTOLEMY

A Program for Heavy-ion Direct-reaction Calculations

by

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and Steven C. Pieper

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Physics Division

March 1976

Sophisticated programs contain subtle errors.

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This manual corresponds to the February, 1976, version of Ptolemy. Small improvements to the optical model fitter were made in this version. Several programming errors have been removed from DWBA calculations, but no substantial changes to the specifications of the DWBA part of the program have been made. Significant changes to this manual are marked with a vertical bar (|) in the left margin and should be carefully reviewed.

Ptolemy is still under development and it may be expected that some of the specifications given in this manual will change from time to time without warning.

Contents

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ABSTRACT

Ptolemy is an IBM/360 program for the computation of nuclear elastic and direct-reaction cross sections. It carries out both optical-model fits to elastic-scattering data at one or more energies, and DWBA calculations for nucleon-transfer reactions. Ptolemy has been specifically designed for heavy-ion calculations. It is fast and does not require large amounts of core. The input is exceptionally flexible and easy to use. This report outlines the types of calculation that Ptolemy can carry out, summarizes the formulas used, and gives a detailed description of its input.

I - Introduction

Ptolemy is a program for the computation of the Distorted Wave Born Approximation to nuclear direct-reaction amplitudes. No use is made of approximations that rely on the short range of nuclear interactions (e.g. zero-range and no-recoil approximations). It is specifically designed for heavy ion reactions but is nonetheless very efficient for light ion reactions. Advantages of Ptolemy over other DWBA codes include high speed, low core requirements, and ease of use.

Ptolemy derives its speed and compactness from several design features:

1) Substantial effort has been put into the development of the subroutine that picks the three-dimensional integration grid. This subroutine makes use of the bound state form factor and the properties of the scattering wavefunctions. This efficiently chosen integration grid results in the need for relatively small numbers of integration points; as an example, a grid consisting of 24 X 10 X 10 points will give accuracies of 1 or 2 percent for many heavy ion reactions at moderate energies.

2) Interpolation and extrapolation in L-space is used to reduce the number of radial integrals that must be computed. Interpolation is achieved by fitting a continued fraction to the computed values, while the exponential form of the radial integrals for large L is used for extrapolation. For Oxygen on Lead reactions, a time savings of 90% is realized by this method.

3) The two inner loops of the radial integral computation have been coded in assembly language that is specifically designed for the special features of the 370/195. These loops function some three times faster than the equivalent Fortran-generated code.

4) The calculation of the angular transforms has been implemented using cosines instead of spherical harmonics. In addition, a specially designed in-line cosine routine is used.

5) The program has been factored into segments in such a way that the recomputation of the same quantities is held to a reasonable (although not absolute) minimum without the need for extremely large tables.

6) Ptolemy has been overlaid to about 25% of its unoverlaid size. Nonetheless, overlay thrashing is not excessive and is independent of the size of the calculation. The overlay processing adds an estimated three seconds to a complete calculation.

7) All arrays used in a Ptolemy calculation are stored in a section of core referred to as the allocator. This allocator is obtained at the start of the job from the available core in the region specified on the user's JOB card. Space in the allocator is reused when the data contained in it is no longer needed. Since the allocator size can change from job to job, small calculations may be carried out in small regions while larger calculations are possible without the recompilation of any part of Ptolemy.

The result of these and other features is a very fast program for the non-zero range DWBA. Accurate $^{16}O+^{48}Ca$ calculations at 56 MeV may be carried out in 7 - 15 CPU seconds (on the 370/195) and

200K of core, while the $^{208}Pb(^{16}O,^{15}N)^{209}Bi(7/2^-)$ reaction including both L transfers at 104 MeV requires only 17 seconds and 220K of core. Further time savings may be realized by storing the form factor integrals in a dataset for use in subsequent calculations with different optical potentials.

In addition to its great speed, Ptolemy provides the user with an especially simple form of input. The input is designed to be flexible, tolerant of minor syntactical variations, concise and easy to remember. Extensive checking of the input is carried out in an effort to allow the same problem to be stated in a variety of ways and to eliminate the chance of calculations being made with undefined or otherwise unexpected parameters. In the following sections it will become evident that many quantities may be defined in more than one way. Often there will be the possibility of a direct specification of a parameter that can also be determined by Ptolemy from other input. In most cases if the user explicitly specifies the value, Ptolemy will not use the indirectly specified value nor will it check the two values for consistency. Therefore one should avoid needless duplication of input so that inadvertant inconsistencies do not occur. An example would be the specification of Q after the bound state calculations - the new value of Q would be used in determining the outgoing state scattering energy even though it might be inconsistent with the difference of the bound state energies.

Provision is made for keeping final results (radial integrals, elastic S-matrix elements, differential cross sections, etc.) in a form suitable for subsequent processing with Speakeasy+. This is particulary useful for the production of graphs showing the results of one or more DWBA calculations. In addition one may use the extensive facilities of Speakeasy to manipulate cross sections or radial integrals interactively.

In addition to the computation of DWBA cross sections, Ptolemy can also be used to fit optical potentials to elastic scattering data. The specification of the parameters to be varied is both simple and flexable; the user does not need to write a subroutine for each fit to be made. The method of entering data is quite general; if the user's data is already punched on cards for a different fitter, he will probably not need to repunch it for Ptolemy. Fits to data at several energies may be made, and several keywords are provided to give the optical potential a dependance on the scattering energy. The user is given a choice of five different minimum-search programs including one that uses analytically computed gradients. The latter fitter works exceptionally well and 12-parameter fits to $^{16}O+^{208}Pb$ data at five different energies may be made in less than a minute of /195 time.

+ S. Cohen, "The Speakeasy-3 Reference Manual," Argonne National Laboratory Report ANL-8000, 1973.

In the next section we discuss the notation of the DWBA formalism while the syntax used in Ptolemy's input is described in Sec. III. Sec. IV shows how one defines the physical problem to be solved while Sec V deals with the choice of the integration grids and related matters. In Sec. VI we show how some of the subroutines of Ptolemy may be used in calculations other than DWBA calculations. Section VII descibes the optical model potential fitter. Section VIII presents some of the control keywords that perform functions auxilary to the calculational functions. Appendix A contains a complete list of Ptolemy keywords and their default values. Appendix B provides core and run time estimates. Appendix C shows the JCL needed to use Ptolemy at Argonne and Appendix D contains the complete input decks for some sample jobs.

This manual does not enumerate all possible variants and interpretations of the Ptolemy input; rather it is limited to the most straightforward methods of stating the problem to be solved. For many DWBA calculations and optical-model fits, the necessary input can be inferred directly from the examples given in Appendix D, to which the tyro is referred. The only aspect of the input that is not clear upon inspection of these examples is the use in DWBA calculations of the PARAMETERSET keyword which is discussed on page 36.

II. Statement of the Physical Problem and Summary of Formulas

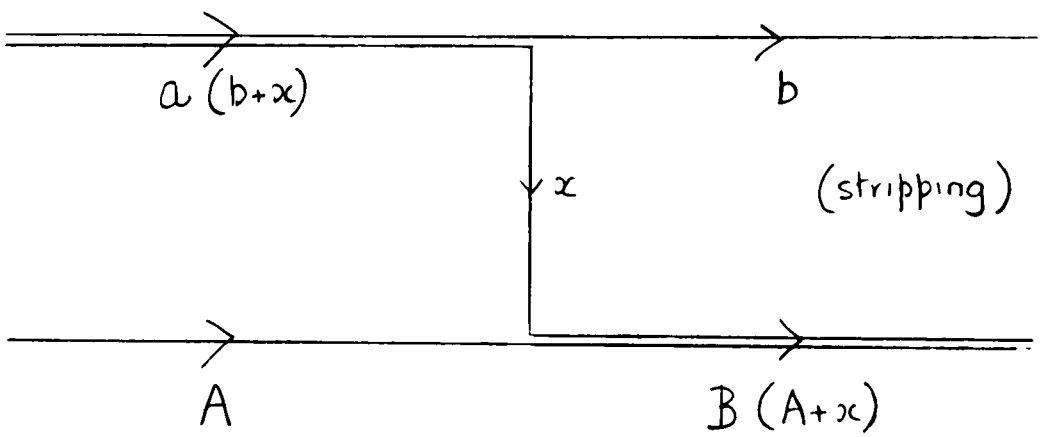
Ptolemy computes amplitudes and cross sections of nucleon-transfer reactions

$$A\,(a,b)\,B \tag{II.1}$$

using the full distorted-wave Born approximation[†] (DWBA), without further approximations based on the short range of nuclear interactions. In the incoming channel (A,a), A is the target and a is the projectile; in the outgoing channel (B,b), B is the residual nucleus and b the ejectile. A, a, B, b will be used both as identifiers of the nuclear states involved and as symbols for the total numbers of nucleons. The group of nucleons transferred (or the number of transferred nucleons) will be denoted by x.

Possible Reactions

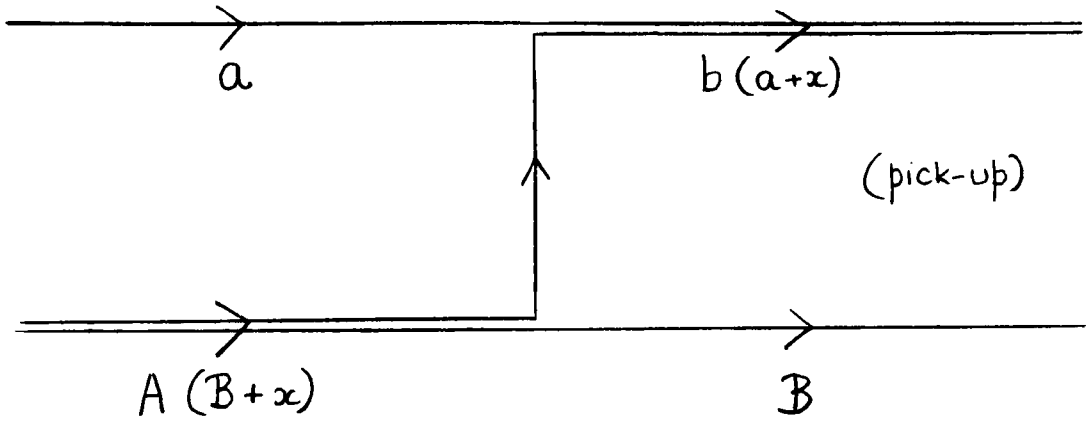
(i) If a > b, the reaction (II.1) is a stripping reaction.



$$\begin{aligned} a &= b + x \\ B &= A + x \end{aligned} \quad \text{(stripping)} \tag{II.2}$$

[†] G. R. Satchler, in Lectures in Theoretical Physics. Vol. VIIIc (Univ. of Colorado press, Boulder, 1966).
N. Austern, Direct Nuclear Reaction Theories (Interscience. New York, 1970).

(ii) If a < b, the reaction (II. 1) is a pick-up reaction.



$$b = a + x \quad (\text{pick-up})$$
$$A = B + x \qquad \text{(II. 3)}$$

Two-Body States

Calculation of the transfer cross sections involves the combination of four elements—the scattering wave functions in incoming (i) and outgoing (out) channels and bound-state wave functions representing the composite nucleus at each reaction vertex. The vertex involving A, B and x will be referred to as the target vertex and the corresponding bound state as the target bound state; the vertex involving a, b and x will be referred to as the projectile vertex and the corresponding bound state the projectile bound state.

The Q value of the reaction is defined by

$$Q = \mathcal{E}_B + \mathcal{E}_b - \mathcal{E}_A - \mathcal{E}_a \qquad \text{(II. 4)}$$

where the $\mathcal{E}_k$ are the total energies (in MeV) of the nuclear states involved;

$$\mathcal{E}_k = (Z_k M_p + N_k M_n)c^2 + (M_{xc})_k + E_k^* \qquad \text{(II. 5)}$$

or

$$\mathcal{E}_k = E_g(Z_k, N_k) + E_k^* \qquad \text{(II. 6)}$$

Z_k, N_k are the numbers of nucleons in the nuclear state k, $(Mxc)_k$ is the ground-state mass excess of the nucleus with Z_k protons and N_k neutrons and E_k^* is the excitation energy if state k is excited. $E_g(Z_k, N_k)$ is the total ground-state energy (or mass $\times c^2$) of the nucleus (Z_k, N_k). When nuclear masses occur in the calculation of momenta from kinetic energies, minor effects such as excitation energies and the n-p mass difference are ignored; in such cases the mass numbers are used as the nuclear masses in a.m.u. ($M_A = A$, etc.).

Consider first the specification of the scattering wave functions in incoming and outgoing channels.

(i) Incoming Channel: i = (A,a)

The center-of-mass kinetic energy is

$$E_i = \left[\frac{M_A}{M_A + M_a}\right] E_{LAB} \qquad \text{(II. 7)}$$

where E_{Lab} is the laboratory kinetic energy of the incoming projectile. The relative momentum is

$$c\hbar k_i = \left[2 M_i E_i\right]^{1/2} \qquad \text{(II. 8)}$$

where M_i is the reduced mass in MeV/c^2:

$$M_i = \frac{M_A M_a}{M_A + M_a} m_0 \qquad \text{(II. 9)}$$

with the atomic mass unit m_0 given in (II. 65). The wave number is k_i.

Let $\vec{r}_i$ be the position vector of the mass center of a relative to that of A; $\vec{L}_i$ is the corresponding relative orbital angular momentum operator

$$\vec{L}_i = \vec{r}_i \times (\hbar \vec{k}_i). \qquad \text{(II. 10)}$$

Then the optical-model scattering wave function in channel i is

$$\chi^+(\vec{k}_i, \vec{r}_i) = \frac{4\pi}{k_i r_i} \sum_{L_i} i^{L_i} f_{L_i}(k_i r_i) \left(Y^{L_i}(\hat{r}_i) \cdot Y^{L_i}(\hat{k}_i)\right) \qquad \text{(II. 11)}$$

$Y^L_M(\hat{r})$ is the spherical harmonic of the unit vector $\hat{r}$. $f_L(kr)$ is the solution of the radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} + \left(k^2 - \frac{2MV(r)}{\hbar^2} - \frac{L(L+1)}{r^2}\right)\right] f_L(kr) = 0 \qquad \text{(II.12)}$$

with the asymptotic behavior and normalization

$$f_L(kr) \xrightarrow[r\to\infty]{} \frac{1}{2}\left[(1+S_L)F_L(kr) + i(1-S_L)G_L(kr)\right] \qquad \text{(II.13)}$$

where F_L and G_L are regular and irregular Coulomb functions.† The elastic S-matrix element S_L is defined by (II.13).

(ii) Outgoing Channel: out = (B, b)

The center-of-mass kinetic energy in the outgoing channel is

$$E_{out} = E_i + Q \qquad \text{(II.14)}$$

and the outgoing relative momentum is

$$c\hbar k_{out} = \left[2M_{out}E_{out}\right]^{1/2} \qquad \text{(II.15)}$$

with the reduced mass given by an equation similar to (II.9).

Let $\vec{r}_{out}$ be the position vector of the center of mass of b relative to that of B; $\vec{L}_{out}$ is the corresponding orbital angular momentum operator

$$\vec{L}_{out} = \vec{r}_{out} \times (\hbar\vec{k}_{out}). \qquad \text{(II.16)}$$

The outgoing-channel optical-model wave function is given in the form

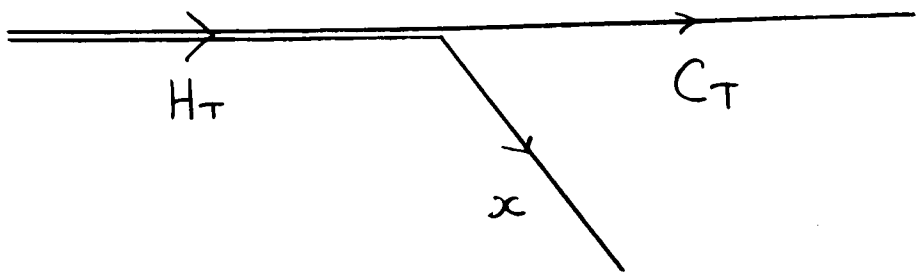
$$\left[\chi^-(\vec{k}_{out}, \vec{r}_{out})\right]^* = \frac{4\pi}{k_{out}r_{out}} \sum_{L_{out}} i^{-L_{out}} f_{L_{out}}(k_{out}r_{out}) \left(Y^{L_{out}}(\hat{r}_{out}) \cdot Y^{L_{out}}(\hat{k}_{out})\right) \qquad \text{(II.17)}$$

† M. Abramovitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1965).

where the radial wave functions satisfy equations analogous to (II. 12) and (II. 13).

Consider next the interaction vertices.

(iii) The Target Vertex: $T = (x, C_T)$



Let C_T denote the core nucleus and H_T the composite (heavier) nucleus at the target vertex

$$\begin{aligned} C_T &= B \text{ (pick-up)} \qquad & H_T &= A \text{ (pick-up)} \\ &= A \text{ (stripping)} & &= B \text{ (stripping)}. \end{aligned} \tag{II. 18}$$

In either case vertex T is regarded as the break-up of the bound state H_T into its constituents

$$H_T \longrightarrow C_T + x. \tag{II. 19}$$

The radial variable associated with this break-up is

$$\begin{aligned} \vec{r}_T = \vec{r}_{C_T x} &= \vec{r}_{Bx} \text{ (pick-up)} \\ &= \vec{r}_{Ax} \text{ (stripping)}. \end{aligned} \tag{II. 20}$$

Introduce a complete set of states

$$\varphi^{n_T \ell_T}_{m_T}(\vec{r}_T) = R_{n_T \ell_T}(r_T)\, Y^{\ell_T}_{m_T}(\hat{r}_T) \tag{II. 21}$$

describing the radial bound-state wave-function of x and C_T. Let the transferred nucleons have intrinsic spin J_x and internal quantum numbers x.†

†Also used for the number of transferred nucleons!

The particles emitted (or absorbed) at vertex T are described in terms of the functions

$$\left[\varphi^{n_T \ell_T}(\vec{r}_T) \times \Phi^{x J_x}(\xi_x)\right]^{J_T}_{M_T} . \qquad \text{(II. 22)}$$

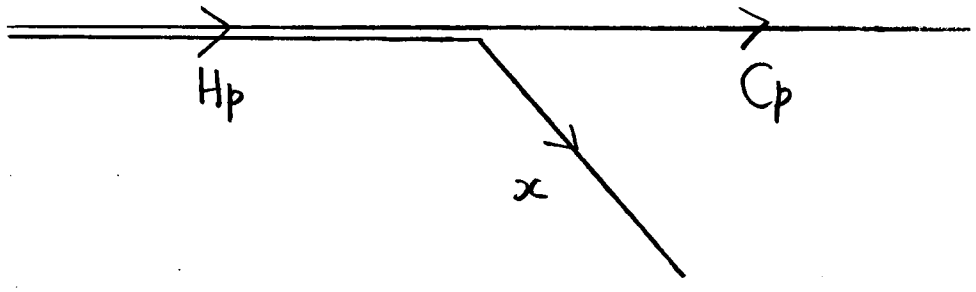
The break-up of the internal wave function of H_T into $C_T + x$ is to be described in terms of shell-model wave functions. This is characterized by a spectroscopic amplitude $\Theta(n_T \ell_T, x J_x, J_T; H_T, C_T)$ defined below [(II.61), (II. 62)]. The coupling schemes for the angular momenta at vertex T are

$$\vec{\ell}_T + \vec{J}_x = \vec{J}_T \qquad \text{(II. 23)}$$

$$\vec{J}(C_T) + \vec{J}_T = \vec{J}(H_T) \qquad \text{(II. 24)}$$

Equation (II. 24) defines the total angular momentum J_T transferred at vertex T; eq. (II. 23) specifies how J_T is divided into orbital and intrinsic components.

(iv) Projectile Vertex: $p = (x, C_p)$



As in the treatment of the target vertex, C_p denotes core, H_p composite (heavier) nucleus.

$$\begin{aligned} C_p &= a \text{ (pick-up)} & H_p &= b \text{ (pick-up)} \\ &= b \text{ (stripping)} & &= a \text{ (stripping)}. \end{aligned} \qquad \text{(II. 25)}$$

Thus vertex p describes the break-up of the bound state H_p into its constituents

$$H_p \longrightarrow C_p + x. \tag{II.26}$$

The radial variable is

$$\vec{r}_p = \vec{r}_{C_p x} = \vec{r}_{ax} \text{ (pick-up)} = \vec{r}_{bx} \text{ (stripping)}. \tag{II.27}$$

The equations describing the state of the particles emitted (or absorbed) at p are obvious analogs of (II.21), (II.22). The equations analogous to (II.23), (II.24) for the angular momentum $\vec{J}_p$ transferred at vertex p are:

$$\vec{\ell}_p + \vec{J}_x = \vec{J}_p \tag{II.28}$$

$$\vec{J}(C_b) + \vec{J}_p = \vec{J}(H_b) \tag{II.29}$$

Vector Transformation between Bound-State and Scattering Variables

Ignoring for the moment the internal structure of the nuclear states C_p and C_T, the transfer reactions under consideration are (x+2)-body processes—the "bodies" are the two cores and the x transferred nucleons. Now let the effective interaction that induces transfer be taken to be a function of the bound-state variables $\vec{r}_p, \vec{r}_T$ only; i.e., it is independent of the internal coordinates ξ_x of x, dependent only on the position of the mass center of the x transferred nucleons. The (x+2)-body process now becomes a 3-body process (C_p, C_T and x).

The natural variables for this 3-body problem are the position vectors of C_p, C_T and x relative to an origin fixed in space. In order to separate the center-of-mass motion, introduce as independent variables the c.m. position vector $\vec{R}$ and two (any two) of the relative variables $\vec{r}_i, \vec{r}_{out}, \vec{r}_T, \vec{r}_p$. Ptolemy uses the scattering variables ($\vec{r}_i, \vec{r}_{out}$) as integration variables. The Jacobian of the transformation

$$(\vec{R}_{C_T}\ \vec{R}_{C_p}\ \vec{R}_x) \longrightarrow (\vec{R}, \vec{r}_i, \vec{r}_{out}) \tag{II.30}$$

is

$$\left.\begin{aligned} \mathcal{J} &= \alpha^3 \\ \text{where} \quad \alpha &= \frac{H_p H_T}{(C_p + C_T + x)\, x} \end{aligned}\right\} \qquad \text{(II. 31)}$$

and is included in the expression (II. 32) for the transformation function $\mathcal{H}$.

With $\vec{r}_i$, $\vec{r}_{out}$ as independent variables, angular-momentum functions of $\vec{r}_p, \vec{r}_T$ must be expressed in terms of $\vec{r}_i, \vec{r}_{out}$. This involves evaluation of the coefficients $\mathcal{H}^{n_T \ell_T n_p \ell_p}_{L_i L_{out} L_x}(r_i, r_{out})$ of the vector transformation

$$\alpha^3 R_{n_T \ell_T}(r_T)\, V_{eff}\, R_{n_p \ell_p}(r_p) \left[Y^{\ell_T}(\hat{r}_T) \times Y^{\ell_p}(\hat{r}_p) \right]^{L_x}_{M_x}$$

$$= \sum_{L_i L_{out}} \mathcal{H}^{n_T \ell_T\, n_p \ell_p}_{L_i\, L_{out}\, L_x}(r_i, r_{out}) \left[Y^{L_i}(\hat{r}_i) \times Y^{L_{out}}(\hat{r}_{out}) \right]^{L_x}_{M_x} \qquad \text{(II. 32)}$$

of the bound-state product into spherical harmonics of the independent variables $\vec{r}_i, \vec{r}_{out}$. Here V_{eff} is the effective interaction that induces the transition. It will be defined below [(II. 49), (II. 50)]; all that is of consequence here is that V_{eff} depends only on the radial variables. $\mathcal{H}(r_i, r_{out})$ is referred to as the bound-state form factor.

Calculation of Bound-State Form Factor

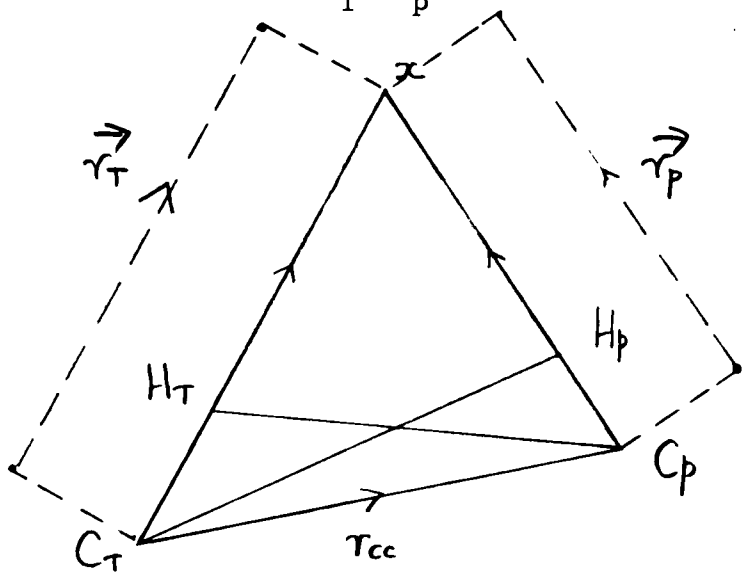
The radial bound-state wave functions $R_{n\ell}(r)$ are eigenfunctions of potentials (including spin-orbit components) whose depths are adjusted to reproduce the empirical separation energies at the two vertices. The procedure for computation of the form factor $\mathcal{H}$ in (II. 32) is that of Balian and Brézin.†

†R. Balian and E. Brézin, Nuovo Cimento 61B, 403 (1969).

First, $\vec{r}_T$ and $\vec{r}_p$ must be expressed in terms of $\vec{r}_i$ and $\vec{r}_{out}$

$$\begin{pmatrix} \vec{r}_T \\ \vec{r}_p \end{pmatrix} = \begin{bmatrix} s_1 & t_1 \\ s_2 & t_2 \end{bmatrix} \begin{pmatrix} \vec{r}_i \\ \vec{r}_{out} \end{pmatrix}. \qquad \text{(II. 33)}$$

To identify the constants s_i, t_i consider the plane triangle whose vertices are the three basic particles C_T, C_p and x.



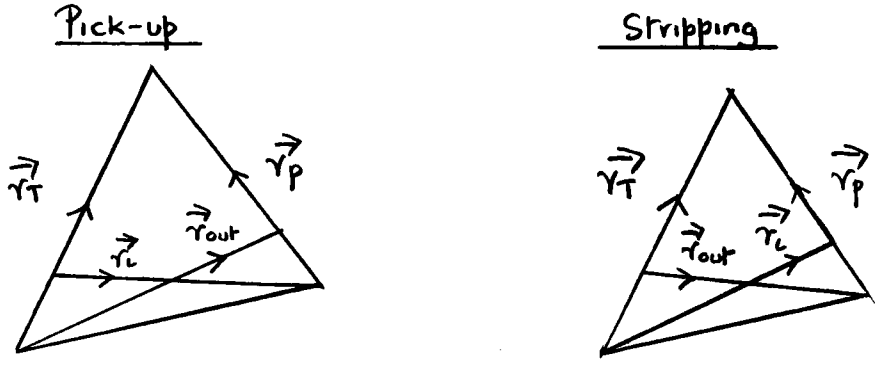
H_T and H_p are at the mass centers of (C_T, x) and (C_p, x). The vectors $\vec{r}_i$ and $\vec{r}_{out}$ have different identifications for pickup and stripping:

Pickup

$$\left.\begin{aligned} \vec{r}_i &= \vec{r}_{Aa} = \vec{r}_{H_T C_p} \\ \vec{r}_{out} &= \vec{r}_{Bb} = \vec{r}_{C_T H_p} \end{aligned}\right\} \qquad \text{(II. 34)}$$

Stripping

$$\left.\begin{aligned} \vec{r}_i &= \vec{r}_{Aa} = \vec{r}_{C_T H_p} \\ \vec{r}_{out} &= \vec{r}_{Bb} = \vec{r}_{H_T C_p} \end{aligned}\right\} \qquad \text{(II. 35)}$$



Then with α defined by (II. 31) and

$$\gamma = \frac{C_p}{H_p} \qquad \delta = \frac{C_T}{H_T} \tag{II. 36}$$

$$\left.\begin{aligned} \begin{bmatrix} s_1 & t_1 \\ s_2 & t_2 \end{bmatrix} &= \alpha \begin{bmatrix} -\gamma & 1 \\ -1 & \delta \end{bmatrix} \text{ (pick-up)} \\ &= \alpha \begin{bmatrix} 1 & -\gamma \\ \delta & -1 \end{bmatrix} \text{ (stripping)} \end{aligned}\right\} \tag{II. 37}$$

The bound-state form factor is then given by

$$\mathcal{H}^{n_T \ell_T \, n_p \ell_p}_{L_i L_{out} L_x}(r_i, r_{out}) = \alpha^3 \int_{-1}^{1} dx \cdot$$

$$\times A_{12}(\ell_T \ell_p L_i L_{out} L_x ; x)\left[R_{n_T \ell_T}(r_T(x)) \; V_{eff} \; R_{n_p \ell_p}(r_p(x))\right] \tag{II. 38}$$

where

$$x = \cos\varphi = \hat{r}_i \cdot \hat{r}_{out} \tag{II. 39}$$

and r_T, r_p are functions of x through

$$r_T(x) = \left[s_1^2 r_i^2 + t_1^2 r_{out}^2 + 2 s_1 t_1 r_i r_{out} x\right]^{1/2}$$
$$r_p(x) = \left[s_2^2 r_i^2 + t_2^2 r_{out}^2 + 2 s_2 t_2 r_i r_{out} x\right]^{1/2} \qquad \text{(II. 40)}$$

The angular factor A_{12} in (II. 38) is:

$$A_{12}(\ell_T \ell_p L_i L_{out} L_x; x) = -\frac{1}{2}(-)^{L_i + L_{out} + \ell_p - \ell_T}\left[(2L_i+1)(2L_{out}+1)(2\ell_T+1)(2\ell_p+1)\right]^{1/2}$$

$$\times \sum_{M_x \mu m} \begin{pmatrix} \ell_T & \ell_p & L_x \\ m & M_x - m & -M_x \end{pmatrix} \begin{pmatrix} L_i & L_{out} & L_x \\ \mu & M_x - \mu & -M_x \end{pmatrix} \Lambda^{\ell_p}_{M_x - m} \Lambda^{\ell_T}_{m} \Lambda^{L_i}_{\mu} \Lambda^{L_{out}}_{M_x - \mu}$$

$$\cos\left(m\phi_T + (M_x - m)\phi_p - \mu\phi\right) \qquad \text{(II. 41)}$$

where ( ) are 3j-symbols, φ is defined by (II. 39) and

$$\phi_T = (-)^{\mathcal{S}} \cos^{-1}\left(\hat{r}_T \cdot \hat{r}_{out}\right) = (-)^{\mathcal{S}} \cos^{-1}\left[\frac{s_1 r_i x + t_1 r_{out}}{r_T}\right]$$
$$\phi_p = (-)^{\mathcal{S}} \cos^{-1}\left(\hat{r}_p \cdot \hat{r}_{out}\right) = (-)^{\mathcal{S}} \cos^{-1}\left[\frac{s_2 r_i x + t_2 r_{out}}{r_p}\right] \qquad \text{(II. 42)}$$

In the above φ and $\cos^{-1}$ are between 0 and π and

$$(-)^{\mathcal{S}} = -1 \quad \text{(pick-up)}$$
$$= +1 \quad \text{(stripping)}. \qquad \text{(II. 43)}$$

Finally,

$$\Lambda^k_q = 0 \quad \text{if } k \pm q \text{ is odd}$$
$$= (-)^{\frac{k+q}{2}} \frac{\left[(k+q)!\,(k-q)!\right]^{1/2}}{2^k \left(\frac{k+q}{2}\right)!\left(\frac{k-q}{2}\right)!} \quad \text{if } k \pm q \text{ is even.} \qquad \text{(II. 44)}$$

DWBA Amplitude and Effective Interaction

The transfer amplitude in DWBA has the form

$$T(\vec{k}_i \to \vec{k}_{out}) = \mathcal{J} \iint d^3r_i \, d^3r_{out} \left[\chi^-(\vec{k}_{out}, \vec{r}_{out})\right]^* \langle B,b|V_{eff}|A,a\rangle \chi^+(\vec{k}_i, \vec{r}_i) \quad \text{(II. 45)}$$

where $\langle V_{eff} \rangle$ denotes a matrix element with respect to all internal core coordinates; $\langle V_{eff} \rangle$ is a function of $\vec{r}_T$ and $\vec{r}_p$. The transition operator V_{eff} is the part of the sum of two-body interactions between constituents of the colliding species in either channel that is not contained in the optical potential in that channel. According to (II. 34), (II. 35):

$$\left.\begin{aligned} V_{eff} &= \sum_{i \in C_p} \sum_{j \in H_T} V_{ij} - U_{opt}(r_{C_p H_T}) \\ \text{or} \\ V_{eff} &= \sum_{i \in C_T} \sum_{j \in H_p} V_{ij} - U_{opt}(r_{C_T H_p}). \end{aligned}\right\} \quad \text{(II. 46)}$$

Two standard approximations are then made.

(i) The additional particles x have little influence on the core-core optical potential. U_{opt} thus describes the core-core interaction.

$$U_{opt} \simeq \sum_{i \in C_p} \sum_{j \in C_T} V_{ij} \quad \text{(II. 47)}$$

and thus

$$\left.\begin{aligned} V_{eff} &\simeq \sum_{i \in C_p} \sum_{j \in x} V_{ij} \\ \text{or} \\ V_{eff} &\simeq \sum_{i \in C_T} \sum_{j \in x} V_{ij} \end{aligned}\right\}. \quad \text{(II. 48)}$$

(ii) The sum of two-body interactions $\sum_{i\epsilon C}\sum_{j\epsilon x} V_{ij}$ is replaced by a one-body potential $V(\vec{r}_{Cx})$ depending only on the relative position of the mass center of x to that of the core

$$\left.\begin{aligned} V_{eff} &\simeq V_{C_p x}(r_p) \\ \text{or} \quad V_{eff} &\simeq V_{C_T x}(r_T). \end{aligned}\right\} \qquad \text{(II. 49)}$$

It is the second approximation that reduces x-nucleon transfer to a three-body problem.

In the simplified form (II. 49) V_{eff} can be associated with one or the other vertex. For the one-body potential V_{Cx}, Ptolemy uses the potential that binds the composite system H at the appropriate vertex.

It is known that the approximation (II. 47) is poor for the Coulomb part of the interaction. In this case a simple correction[†] can be made;

$$\begin{aligned} V_{eff} &\simeq V_{C_p x}(r_p) + \Delta V^C \\ \text{or} \quad V_{eff} &\simeq V_{C_T x}(r_T) + \Delta V^C \end{aligned} \qquad \text{(II. 50)}$$

where

$$\Delta V^C = V^C(r_{cc}) - V^C_{opt}. \qquad \text{(II. 51)}$$

In (II. 51), V^C indicates the one-body Coulomb potential given in Sec. IV-B; $V^C(r_{cc})$ is the Coulomb interaction between the cores and V^C_{opt} the Coulomb part of the appropriate optical potential as indicated in the table.

	Pick-up	Stripping
Interaction at p Vertex	$V^C_{opt}(r_i)$	$V^C_{opt}(r_{out})$
Interaction at T Vertex	$V^C_{opt}(r_{out})$	$V^C_{opt}(r_i)$

With the Coulomb correction ΔV^C, V_{eff} becomes a function of r_p, r_T and x in a fashion which adds no essential complication to the integral in (II. 38).

[†] R. M. deVries, G. R. Satchler and J. G. Cramer, Phys. Rev. Letters 32, 1377 (1974).

In Ptolemy, the following options are available for V_{eff}.

i) V_{eff} can be associated with either vertex.

ii) a) Only the nuclear part of the binding potential V_{cx} may be used.

b) Both nuclear and Coulomb parts of the binding potential may be included.

c) The core-Coulomb correction (II. 51) may be added to b).

The default option is to include the Coulomb corrections and to associate the interaction with the projectile vertex.

Angular Momenta

The angular momenta transferred at the vertices, J_T and J_p have been defined in eqs. (II. 24) and (II. 29). The total transferred angular momentum L_x is defined by

$$\vec{L}_x + \vec{J}_p = \vec{J}_T. \qquad \text{(II. 52)}$$

The multipole or angular-momentum decomposition of the DWBA amplitude and cross section is based on the total angular-momentum transfer.

Differential Cross Section (in mb/sr)

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{10}{E_i E_{out}} \cdot \frac{k_{out}}{k_i} \cdot \mathcal{R} \sum_{J_T J_p} \sum_{L_x M_x} \left| G_{M_x}^{L_x (J_T J_p)}(\theta) \right|^2 \qquad \text{(II. 53)}$$

where $\mathcal{R}$ is a spin-statistical factor;

$$\left.\begin{aligned} \mathcal{R} &= \frac{2J_b + 1}{2J_a + 1} \quad \text{(pick-up)} \\ &= \frac{2J_B + 1}{2J_A + 1} \quad \text{(stripping)} \end{aligned}\right\}. \qquad \text{(II. 54)}$$

In Ptolemy only one value of J_T and J_P is allowed and the sum over J_T and J_P in (II. 54) consists of only one term.

Components of Multipole Amplitude

The multipole transition amplitude G is a sum of products of spectroscopic and geometrical components

$$G_{M_x}^{L_x (J_T J_P)}(\theta) = \sum_{n_T \ell_T n_P \ell_P} A_{L_x J_T J_P}(n_T \ell_T n_P \ell_P)\, B_{M_x}^{L_x (J_T J_P)}(n_T \ell_T n_P \ell_P ; \theta) \qquad \text{(II. 55)}$$

summed over all contributing states of orbital motion of the transferred nucleons at each vertex. Ptolemy allows only one projectile and target bound state so the sum in (II. 55) consists of only one term.

(i) Geometrical Component (including radial integrals)

The angular dependence of the cross section is contained in the 'geometrical' component of (II. 55);

$$B_{M_x}^{L_x (J_T J_P)}(n_T \ell_T n_P \ell_P ; \theta) = \sqrt{4\pi}\, i^{L_x + \ell_T - \ell_P} \sum_{L_i L_{out}} C_{M_x - M_x\, 0}^{L_{out}\, L_x\, L_i}\, I_{L_i L_{out} L_x}(n_T \ell_T n_P \ell_P)\, Y_{-M_x}^{L_{out}}(\theta) \qquad \text{(II. 56)}$$

with C a vector-coupling coefficient and θ, the scattering angle, given by

$$\theta = \cos^{-1}\left(\hat{k}_i \cdot \hat{k}_{out}\right). \qquad \text{(II. 57)}$$

The radial integrals are expressed in terms of the bound-state form factor $\mathcal{H}$ [eqs. (II. 38) to (II. 44)] and the radial scattering functions by

$$I_{L_i L_{out} L_x}(n_T \ell_T n_p \ell_p)$$

$$= \iint r_i dr_i \, r_{out} dr_{out} \, f_{L_i}(k_i r_i) \, \mathcal{H}^{n_T \ell_T n_p \ell_p}_{L_i L_{out} L_x}(r_i, r_{out}) \, f_{L_{out}}(k_{out} r_{out}). \tag{II.58}$$

Note that $B^{L_x}_{M_x}$ is independent of the shell-model wave functions of the nuclear states.

(ii) Spectroscopic Factors

Let the states A, a, B, b be represented by shell-model wave functions. In order to treat the center-of-mass variable $\vec{R}$ consistently and to separate internal and center-of-mass variables of the nuclear states, use harmonic-oscillator shell-model wave functions with the center-of-mass motion in its ground (0s) state.

Consider then the internal states at the target vertex. If J_T is the total A.M. transfer at that vertex, let $\underline{\Psi}^{\gamma_T J_T}_{M_T}$ be a complete set of x-nucleon shell-model states for the transferred nucleons, and let $a^\dagger(\gamma_T J_T M_T)$ be the creation operators that produce these states from the vacuum. The x-nucleon states must be projected onto states of the transferred nucleons of the form (II.22), with internal and center-of-mass variables separated. Define the necessary coefficients

$$K_{J_T}(n_T \ell_T \, x J_x ; \gamma_T)$$

$$= \iint d^3R_x \, d^3\xi_x \left(\left[\underline{\phi}^{n_T \ell_T}(\vec{R}_x) \times \underline{\Phi}^{x J_x}(\xi_x) \right]^{J_T}_{M_T} \right)^* \underline{\Psi}^{\gamma_T J_T}_{M_T}(\{\vec{r}_\alpha\}) \tag{II.59}$$

where $\{\vec{r}_a\}$ is a set of nucleon coordinates and

$$\vec{R}_x = \frac{1}{x} \sum_{\alpha=1}^{x} \vec{r}_\alpha . \tag{II.60}$$

Then the conventional spectroscopic amplitude $\sqrt{\mathcal{S}}$ is given by

$$\sqrt{\mathcal{S}(n_T \ell_T, x J_x, J_T; H_T, C_T)}$$

$$= \sum_{\gamma_T} K_{J_T}(n_T \ell_T x J_x; \gamma_T) \langle J(H_T) \| a^\dagger(\gamma_T J_T) \| J(C_T) \rangle \qquad \text{(II. 61)}$$

(The reduced matrix element is defined by the Wigner-Eckart theorem in the form $\langle jm | T^k_q | j'm' \rangle = C^{j'kj}_{m'qm} \langle j \| T^k \| j' \rangle$.)

The treatment of the centers of mass leading to eqs. (II. 59), (II. 61) is exact if the shell-model wave functions and the radial functions Φ in eqs. (II. 21) and its "projectile" analog are harmonic-oscillator functions. However, the radial functions of the target and projectile bound states are eigenfunctions of Woods-Saxon potentials. This difficulty is usually ignored since the level of precision of the entire analysis (in particular of its absolute normalization) is seldom high enough to require consideration of such niceties. A crude correction factor can be introduced by expanding the Woods-Saxon wave functions in terms of oscillator functions and assuming that one term dominates. It can then be shown that the replacement

$$\left.\begin{aligned} \sqrt{\mathcal{S}(n_T \ell_T, x J_x, J_T; H_T C_T)} &\longrightarrow \textcircled{H}(n_T \ell_T, x J_x, J_T; H_T C_T) \\ \textcircled{H}(H_T C_T) &= \left(\frac{H_T}{C_T}\right)^{\frac{2n_T + \ell_T}{2}} \sqrt{\mathcal{S}(H_T C_T)}. \end{aligned}\right\} \qquad \text{(II. 62)}$$

should correct for the use of the oscillator shell-model wave functions. The projectile vertex is handled in the same way.

In Ptolemy, the spectroscopic amplitudes $\textcircled{H}$ are read in directly; they can often be inferred from suitable light-ion reactions between the nuclear states in question. Note that $\mathcal{S}$ as defined above reduces to the standard spectroscopic factor in the case of single-nucleon transfer.

(iii) Spectroscopic Component of the Multipole Transition Amplitude

The spectroscopic component A [eq. (II. 55)] is given in terms of the spectroscopic amplitudes Ⓗ [eqs. (II. 61), (II. 62)] by

$$A_{L_x J_T J_p}(n_T \ell_T n_p \ell_p) = \sqrt{2L_x+1} \cdot \sum_{x J_x} (-)^{J_x - J_p + \ell_p + \ell_T} \times W(\ell_T J_T \ell_p J_p ; J_x L_x) Ⓗ(n_T \ell_T, x J_x, J_T : H_T C_T) Ⓗ(n_p \ell_p, x J_x, J_p : H_p C_p) \quad \text{(II. 63)}$$

A is independent of θ and M_x.

Outline of Steps in a DWBA Computation

The main steps in a DWBA calculation can be schematically summarized as follows. In practice a number of these steps are carried out in parallel.

1) Adjust the potentials at the interaction vertices to reproduce the experimental separation energies and compute the bound-state wave functions. This specifies the effective transition operator through (II. 49) or (II. 50).

2) For given optical-model parameters, solve eqs. (II. 12) for the radial scattering functions. At this stage elastic-scattering amplitudes and cross sections can also be computed.

3) Use eqs. (II. 38) to (II. 44) to compute the bound-state form factors $\mathcal{H}(r_i, r_{out})$.

4) Fold the bound-state form factors with the radial scattering functions and integrate (eq. (II. 58)) to obtain the radial integrals $I_{L_i L_{out} L_x}$.

5) Using given spectroscopic amplitudes Ⓗ compute the spectroscopic components A_{L_x} of the multipole amplitudes using (II. 63).

6) Calculate the geometrical components $B^{L_x}_{M_x}$ of the multipole amplitudes using (II. 56).

7) Construct the multipole components of the transition amplitude using (II. 55) and compute the cross section [eq. (II. 53)].

Note that in heavy-ion calculations, more than 90% of the time is spent carrying out steps (3) and (4)—construction of the bound-state form factors and integration over r_i and r_{out}.

Constants[†]

Ptolemy uses the values:

$$\hbar c = 197.32858 \text{ MeV fm} \tag{II. 64}$$

$$\mathcal{M} = 931.5016 \text{ MeV}/c^2 \tag{II. 65}$$

$$\alpha^{-1} = 137.03604 \tag{II. 66}$$

where $\mathcal{M}$ is the atomic mass unit and α is the fine-structure constant.

[†] E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).

III - Notation and Syntax
A - Notation

Lower case letters cannot be conveniently used as computer input. Thus some changes must be made to the notation established in the previous section. In general lower case letters will simply be converted to upper case. However, in Sec. II a distinction was made between lower- and upper-case letters in the identification of the reaction participants. For Ptolemy input this distinction will be maintained by specifying the target particles as BIGA and BIGB while the projectile particles will be A and B. Thus the reaction computed by Ptolemy may be written as

BIGA(A, B)BIGB .

In the incoming state, the target is referred to as "BIGA" and the projectile is "A". In the final state the residual target is "BIGB" and the ejectile is "B". The exchanged particle is referred to as "X". For a stripping reaction we have

A = B + X,
BIGB = BIGA + X,

while for a pickup reaction

B = A + X,
BIGA = BIGB + X.

Ptolemy will compute either pickup or stripping reactions; it is not necessary for the user to interchange particles to force the reaction into one form or the other. The reaction must actually involve the exchange of mass so that X must have non-zero mass. Furthermore the charge of X may not be negative.

The projectile or ejectile bound state (whichever is appropriate) is always referred to as the projectile bound state while the target or residual nucleus bound state is called the target bound state. The Q value of the reaction is the difference of the outgoing and incoming kinetic energies in the center of mass system so that in terms of the bound state energies

Q = E(projectile) - E(target) : stripping,
Q = E(target) - E(projectile) : pickup.

Note that Ptolemy deals with actual bound state energies (i.e., negative numbers).

The coordinate vector for the projectile bound state is Rp while that of the target bound state is Rt. The coordinate vector for the incoming scattering state is Ri while that of the outgoing state is Rout. The angle between Ri and Rout is PHI. As will be described in more detail later, Ptolemy performs its integrations on the three-dimensional grid (Ri+Rout) X (Ri-Rout) X PHI.

B - Ptolemy Syntax

Ptolemy uses a free-form keyword-based input. Options are specified and stages of the calculation selected by the specification of the appropriate keyword. Data values are entered by the specification of a data keyword followed by the desired data value. One or more keywords and associated data values may be included on a single input line+ or a data value may be on the line following its keyword. (The CHANNEL, REACTION and HEADER keywords are exceptions and require associated data values to be on the same input line.) Keywords and individual data values may not be split across two lines. In both TSO and batch usage, Ptolemy uses only the first 72 positions of the input line; the last 8 are reserved for optional line numbers that will be printed but otherwise ignored.

Keywords may be separated from other keywords on the same line by blanks, commas, or sequences of blanks and commas. The equal sign may be used (but is not required) between a keyword and its associated data value. The colon may be used following the CHANNEL, REACTION and HEADER keywords but should not otherwise be used in Ptolemy input. The semicolon is used to begin a stage of the calculation; it indicates that all input needed for that stage has been provided.

Numerical data may be entered with or without a decimal point and may have the E or D form of exponent. Valid numerical inputs are

2, 2.3, .0002, 2D-4, 2.325E+7, -5.3, +7E-5 .

An "E" or "D" appearing in a number indicates the beginning of the power of 10 bywhich the number is to be multiplied. Thus

$5.3E-7 = 5.3 \times 10^{-7}$

$1D20 = 10^{+20}$

Angular momenta that have the possibility of being half-integer (J or S values but not I values) have a special form of input. They may be either simple integers or integers followed by "/2" to indicate half integer values. They should not be coded with a decimal point. Thus

J = 2, S = 3/2, JP = 4/2

are all valid (the last is the same as JP = 2) while

J = 2., S = 1.5

are both invalid. Such J and S values may be followed by a parity sign which will be ignored. Thus

J = 2, J = 2-, and J = 2+

are all equivalent.

Keywords may have more than eight characters in their names but only the first 8 characters are used and required. Keywords never have embedded blanks in their names.

Comments may be placed anywhere in the input. They are

+ Input lines are either cards in an input deck for a batch run or lines typed at a terminal in TSO usage of Ptolemy.

preceded by a dollar sign ($) which indicates that the rest of the input line is a comment. If a second dollar sign appears on the same line, the comment is terminated and the remainder of the line is processed as normal input.

IV - Specifying the Physical Problem
A - Defining the Reaction Participants and Energy

In a standard Ptolemy run the input will be in the following order:

1) Masses, charges, etc., of the 5 particles.
2) Potentials for the two bound states.
3) Optical potentials for the two scattering states.
4) Integration grid specifications and L-value ranges.

Variations on this order are possible; the two most likely are to include item 4) with item 1), and the elimination of items 1), 2) and 4) for a calculation using previously computed form factor integrals.

In more detail a typical Ptolemy input deck will look like

```
reaction definition, ELAB = ...
PROJECTILE   projectile bound state parameters ;
TARGET       target bound state parameters ;
INCOMING     incoming optical parameters  ;
OUTGOING     outgoing optical parameters  ;
grid parameters, L and angular ranges, etc, ;
```

Here the keywords PROJECTILE, TARGET, INCOMING, and OUTGOING indicate which potential parameters are being entered. The semicolons indicate that the complete potential has been defined and that Ptolemy is to go ahead with that stage of the computation (the semicolons are actually part of the input). The final semicolon indicates that all of the computational parameters have been entered and that the DWBA calculation should begin. Of course each of the potential specifications will in general require more than one input line.

The easiest way to define the participants in the reaction is to use the REACTION keyword. This keyword is followed by the statement of the reaction in standard nuclear terminology. Some examples will best illustrate the possibilities:

```
REACTION:  48CA(16O, 14C)50TI
REACTION = 208PB(O16,15N)BI209(7/2- .90)
REACTION   PB208(O16 15N(5/2, 5.27055))BI209
REACTION   PB208(16O(2,6.93) 12C)PO212
```

All four participants must be included in the REACTION specification. They are defined by an element symbol consisting of the atomic number and a one or two- character element abbreviation. The atomic number may either precede or follow the symbol but no blank spaces or other punctuation may intervene. Excited states may be indicated by enclosing the spin and excitation energy in parentheses following the element symbol. The left parenthesis for excited state specification must immediately follow the element symbol. An excited state of the initial target may <u>not</u> be given in this manner, but any or all of the other three particles may have excited state descriptors. The excitation energy and spin of the excited state may be given in either order, and the excitation energy must include a decimal point even if it happens to be an

integer. Excitation energies are given in MeV. The complete reaction specification must be on the same input line as the REACTION keyword. Except as has been otherwise indicated, blank spaces and commas may be freely used to make the reaction specification more readable.

The REACTION keyword results in the definition of the atomic mass and charge of the four particles. The atomic mass and charge of the exchanged particle is then computed by subtraction. The 1975 Oak Ridge Atomic Mass Adjustment and the 1971 Nuclear Wallet Cards compilation+ is then used to find the ground state mass excesses and spins of all 5 particles. The ground state mass excesses (along with the excitation energies, if given) will be used during the bound state computation to find the separation energies of the exchanged particle (X) from the appropriate cores.

Individual data values defined by the REACTION keyword may be overriden by the use of other keywords or the REACTION keyword may be omitted and all of the particle definitions entered via other keywords. The keywords that define the five particles have the form "Ki" where "K" indicates what quantity is being defined and "i" is a suffix indicating which particle is involved (BIGA, A, B, BIGB, or X). The possibilities for K are

M - The mass in AMU. This need not be an integer.
Z - The charge.
J - The spin of the nucleus.
MXCG - The mass excess of the ground state.
E* - The excitation energy in MeV.
MXC - The mass excess of the nucleus (MXCi = MXCGi + E*i).

As an example

MB=15, ZB=7, JB=5/2, E*B=5.27055, MXCGB = .10152

would define the excited state of ^{15}N contained in the third REACTION example given above. (Alternatively one could have entered MXCB = 5.37207 and left out the E*B and MXCGB keywords or one could directly enter the proton separation energy at the time of the ^{16}O bound state calculation and leave out all the mass excess specifications.) In the following example

REACTION: 209BI(16O 12C)213AT, JBIGB = 9/2

one is supplying the ground state spin of ^{213}At which is not in the the Nuclear Wallet Cards.

The scattering energy is entered by either of the keywords ELAB or ECM followed by the energy in MeV. In both cases the energy refers to the incident kinetic energy; the outgoing energy is determined from the Q value of the reaction.

The Q value may be entered by using the keyword Q followed by the value in MeV. If it is not entered it will be found as the difference of the two bound state energies. If it is entered then it is necessary to define only one of the bound state energies; the other will be found using the Q value. Since the REACTION keyword results in the definition of both bound state energies, it is

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+ F. Serduke, "Atomic Mass Table," Argonne Internal Report, 1975, and private communication.

usually not necessary to enter the Q value.

The version of the DWBA on which Ptolemy is based uses as the effective interaction that induces transfer the potential that binds the composite particle at either the projectile or target vertex. The vertex whose potential is to be used as the effective interaction is specified by the keywords USEPROJECTILE or USETARGET. USEPROJECTILE indicates that the potential for the projectile bound state is the interaction potential; USETARGET causes the target potential to be used. The default is USEPROJECTILE. Note that we avoid the use of the words "post" and "prior" in specifying the interaction vertex.

The content of the interaction potential is controlled with the NUCONLY, USESIMPCOULOMB and USECOULOMB keywords. NUCONLY means that only the nuclear part of the bound state potential is used in the interaction potential (Most published DWBA calculations have used this prescription). USESIMPCOULOMB means that the full bound state potential at the vertex designated by USEPROJECTILE or USETARGET is used. USECOULOMB causes the nuclear potential at the designated vertex to be used with the complete three-body Coulomb potential. The inclusion of the Coulomb corrections due to the third particle removes post/prior descrepancies from the Coulomb part of the interaction and can result in much closer agreement between USETARGET and USEPROJECTILE results. The default is USECOULOMB. Note that DWBA calculations are usually somewhat simpler numerically if the interaction is attached to the vertex (usually the projectile vertex) involving the lighter ions. In a reaction such as $^{208}Pb(^{16}O, ^{17}O)^{207}Pb$ inwhich the projectile and target differ significantly in mass, a USETARGET calculation requires a substantially denser integration grid than is required for USEPROJECTILE.

B - Definition of the Two-Body States

Potential parameters must be entered for each of the two bound states and the two scattering states. The potentials are defined when the bound state or scattering state is to be computed; the same keywords are reused to define the potentials in each of the four states. Each of these four two-body states consists of two particles that are referred to as the "projectile" and "target" (not to be confused with the projectile bound state and target bound state). In the scattering states these words have their normal meanings; for the bound states the exchanged particle (X) is always the "projectile". The suffixes "p" and "t" appearing on some of the symbols in this section refer to "projectile" and "target" respectively.

The potentials are defined by the keywords Vi, Ri or Ri0, and Ai where the suffix "i" indicates the potential that is being defined. Possibilities for "i" are:

1) (null) - no suffix refers to the real part of the Woods-Saxon well.
2) I - The suffix I refers to the imaginary part of the Woods-Saxon well.
3) SO - The suffix SO designates the real part of the spin-orbit force.
4) SOI - Imaginary part of the spin-orbit force.
5) SI - Imaginary surface potential.
6) C - Coulomb potential (only RC and RC0 are defined).

The forms of these potentials are as follows:

1) Real part of the Woods-Saxon:
   $- V / (1 + X)$
   $X = \exp[(r-R)/A]$
2) Imaginary part of the Woods-Saxon (volume absorption):
   $- VI / (1 + XI)$
   $XI = \exp[(r-RI)/AI]$
3) Real part of the spin-orbit:
   $+ (VSO+TAU*V) * 4L\bullet S * (1/r) * (d/dr)\ 1/(1+XSO)$
   $XSO = \exp[(r-RSO)/ASO]$
4) Imaginary part of the spin-orbit:
   $+ (VSOI+TAUI*VI) * 4L\bullet S * (1/r) * (d/dr)\ 1/(1+XSOI)$
   $XSOI = \exp[(r-RSOI)/ASOI]$
5) Imaginary surface potential (surface absorption):
   $+ VSI * 4*ASI * (d/dr)\ 1/(1+XSI)$
   $XSI = \exp[(r-RSI)/ASI]$
6) Coulomb
   $+ Zp*Zt * e^2 / r$: $r \geq RC$
   $+ Zp*Zt * e^2 * \{3 - (r/RC)^2\} / (2RC)$: $r < RC$

where

$$L\bullet S = (Jp(Jp+1) - L(L+1) - Sp(Sp+1)) / 2 .$$

The potential well depths are given in MeV. Note that the spin-orbit well depths may either be specified directly by using the VSO and VSOI keywords or their ratio to the corresponding Woods-Saxon depths may be given by using the TAU and TAUI keywords.

The TAU's are related to the LAMBDA's of DWUCK and LOLA by

TAU = LAMBDA/(4*45.2)

Note that VSO and VSOI have dimensions of MeV since the factor "4" in the definition of the spin-orbit force is interpreted as 2*2 where one "2" converts L•S to L•sigma, and the other "2" is approximately the square of the pion Compton wavelength in fm. The ratio TAU is dimensionless.

In all cases the radius parameter (R0, RI0, RSO0, RSOI0, RSI0 or RC0) may be entered in place of the potential radius. The radius is then computed as

R = R0 * Mt**(1/3) : Mp ≤ 2 ,

R = R0 * { Mp**(1/3) + Mt**(1/3) } : Mp ≥ 3 .

The real and imaginary potential parameters may be given a dependance on the laboratory energy by the use of keywords that end in "E" or "ESQ." In this case the quantities to be used in the above equations will be computed as follows:

A = A + AE*Elab + AESQ*Elab² ,

R0 = R0 + R0E*Elab + R0ESQ*Elab² ,

V = V + VE*Elab + VESQ*Elab² ,

AI = AI + AIE*Elab + AIESQ*Elab² ,

RI0 = RI0 + RI0E*Elab + RI0ESQ*Elab² ,

VI = VI + VIE*Elab + VIESQ*Elab² .

The names appearing on the right of the equal signs in the above equations are the keyword values the user enters. The quantities on the left are then used to evaluate the potentials. The default value for all the keywords ending in "E" or "ESQ" is 0. The laboratory energy corresponding to the outgoing scattering energy is used for the outgoing scattering parameters so that the same keyword values will give slightly different potentials in the incoming and outgoing channels if an energy dependance is specified.

If a given V or TAU is defined in a channel, then its associated R (or R0) and A must also be defined. At the beginning of input for each channel, all V's and TAU's are set to 0 and all R's and A's are undefined. However, R0's and A's will be retained from one bound state to the other and from one scattering state to the other. They will not be retained from bound states to scattering states or vice-versa. The same rules apply to RC and RC0, one of which must be defined if both Zp and Zt are nonzero. If Ai and/or both Ri and Ri0 are not defined for the imaginary part of a potential, Ptolemy will use the Ai or Ri for the real part of the same potential (RSO will be used for RSOI, A for AI, etc.). If ASO or both RSO and RSO0 are not defined, A or R will be used for them. If ASI or both RSI and RSI0 are not defined, AI or RI will be used for them.

The number of nodes and orbital angular momenta of the bound states must be defined when the bound state potentials are specified. The keyword NODES is used to specify the number of nodes. The node at the origin is not included in the count so that the lowest bound state for each value of L has 0 nodes. The keyword "L" is used to specify the orbital angular momentum of the

bound state. If a spin-orbit force is being used in the bound state, it is necessary to enter the total angular momentum of the "projectile". This is done with the keyword "JP." Jp, L and Sp (the spin of the projectile = Jx) are used to find the value of L•S in the above formula (note that Sp is known from the reaction specification). If either of St (the target spin) or J (the total bound state spin) are zero, then Jp need not be specified since it will be uniquely determined by other known spins.

At present spin-orbit forces may not be used in the scattering states of DWBA calculations.

Normally the binding energy (cluster separation energy) of the bound states will be computed by Ptolemy from the information in the REACTION specification. If it is desired to override this bound state energy, one may use the "E" keyword to enter the bound state energy along with the bound state potential. The energy is given in MeV and must be negative for bound states. The "E" keyword may also be used in the scattering state descriptions in which case it specifies the c.m. energy of the state. It will then override the c.m. energy determined from the ELAB keyword or from ELAB combined with the Q value depending on the channel.

In the process of computing the bound state wavefunction it is necessary that V (the potential depth) and E (the bound state energy) be made consistent with each other. Ptolemy varies one or the other of these two quantities until they are consistent. The keywords FITV and FITE may be used to determine which quantity is to be varied. FITV causes V to be changed to produce a well that has the bound state energy E. If a spin-orbit force has been specified via the keyword TAU, the depth of the spin-orbit force is also varied since the ratio of the spin-orbit force to the Woods-Saxon well is held constant at TAU. On the other hand, if VSO is used to specify the spin-orbit force, the strength of the spin-orbit force is not changed as V is changed. FITE causes E to be computed as the bound state energy of the given potential. Use of FITE in DWBA calculations may result in bound state energies (and hence Q-values) that are significantly different from the values determined from the REACTION specification. The default is FITV.

V - Computational Parameters
A - Angular Momentum Ranges

Not all radial integrals used in computing the differential cross sections need be explicitly computed by Ptolemy. Ptolemy will interpolate between computed values and extrapolate beyond the largest value of L for which the radial integrals are computed. The keywords LMIN, LMAX, and LSTEP determine which radial integrals are to be computed. The radial integrals for

Lout = LMIN, LMIN+LSTEP, LMIN+2*LSTEP, ...,

(where the sequence stops at or before LMAX) will be computed. The radial integrals for all Lx and Li associated with these Lout's will be computed. The remaining radial integrals for LMIN ≤ Lout ≤ LMAX will then be found by interpolation using continued fractions. The default value of LSTEP is 1 which causes all radial integrals from LMIN to LMAX to be computed explicitly.

In addition Ptolemy will pick an Lmax' > LMAX such that radial integrals for Li, Lout > Lmax' are negligible. The radial integrals for LMAX < Li, Lout ≤ Lmax' will be found by extrapolation. The extrapolating function used is of Woods-Saxon form in L. Thus LMAX must be sufficently beyond the L-window for such a shape to be an adequate representation of the radial integrals. The keyword MAXLEXTRAPOLATION may be used to limit or completely suppress the extrapolation to L > LMAX. It specifies the maximum allowed Lmax'-LMAX. If it is set to 0, no extrapolation will occur. The default value is 100.

Since no extrapolation to Li, Lout < LMIN is made, LMIN must be small enough to include all important radial integrals. Care should be taken to avoid specifying too small a value of LMIN since the radial integrals for small Li and Lout are small due to extensive cancellations of the integrand viewed as a function of Ri+Rout. In practice these cancellations are hard to reproduce without using a large number of Gauss points and the computed radial integrals may be much larger than they should be. Thus a more accurate solution is often obtained by totally excluding integrals whose contributions are very small but which are hard to calculate accurately.

If LMIN and/or LMAX are not specified, they will be computed as multiples of Lcritical which is estimated via semi-classical expressions. The values of LMIN and LMAX are determined as

LMIN = LMINMULT * Lcritical ,
LMAX = LMAXADD + Lcritical .

The default values of the keywords LMINMULT and LMAXADD are 0.6 and 30 respectively (the LMAXADD default is more appropriate to stand-alone optical model calculations than DWBA calculations). These multipliers and LSTEP are set by the PARAMETERSET keyword (page 37).

For a given reaction there will usually be several possible values of the transfered orbital angular momentum:

Lx = Lout - Li = J(projectile) - J(target) .

Ptolemy will compute the radial integrals for all possible values of Lx and add the resulting cross sections together with the appropriate Racah coefficients. If only one value of Lx is

possible the resulting cross section will still be weighted by the Racah coefficient. If it is desired to have results for only one value of Lx, the keyword LX may be used to specify the desired value. In this case the Racah coefficient and spectroscopic amplitudes or factors (see below) will not be included in the calculation of the cross section. Thus the results will be comparable to those produced by LOLA. Note that different values of the cross section will be produced in problems for which only one Lx is possible depending on whether LX is specified or not.

The spectroscopic amplitudes for the two bound states may be entered with the keywords SPAMP and SPAMT. These amplitudes will be squared and multiplied into the cross sections. The default values are unity. Alternatively the spectroscopic factors (the squares of the amplitudes) may be directly entered using the keywords SPFACP and SPFACT. The spectroscopic factors must be positive.

The grid of c.m. angles on which the differential cross sections are displayed is controlled by the keywords ANGLEMIN, ANLEMAX, and ANGLESTEP. The angles are given in degrees. The default values are

```
ANGLEMIN  =  0 ,
ANGLEMAX  = 90 ,
ANGLESTEP =  1 .
```

The cross sections are given in millibarns/steradian.

B - The Integration Grid

The Ptolemy integration grid is constructed by a rather elaborate set of subroutines consisting of some 1000 Fortran source cards. The construction is fairly automatic and is designed to place the integration points where the integrand is largest. Ideally the user would not have to intervene in this process and would only have to tell the processor the desired accuracy of the final results (the differential cross sections). Unfortunately the subroutine is less than perfect and the user must have some understanding of what the subroutine does. This section describes most of the parameters that control the grid construction. It then introduces the PARAMETERSET keyword which may be used to define frequently-used groups of grid constuction parameters. Eventually the average user will be able to specify his grid by simply using one of these PARAMETERSET keywords but the set of possibilities is presently limited to O+Ca, O+Pb, and closely related reactions.

The Ptolemy integration grid is based on the three variables SUM, DIF, and PHI:

SUM = (Ri + Rout)/2 ,
DIF = Ri - Rout ,
PHI = angle between Ri and Rout.

The numbers of Gauss points in each of these grids is specified by the keywords NPSUM, NPDIF, and NPPHI, respectively. These numbers may have any value between 1 and 2000; typical values will be found in Table I below. The same three-dimensional grid is used for all values of Li, Lout and Lx.

The keyword DWCUTOFF is used in the construction of the integration grids. DWCUTOFF specifies in a relative sense the smallest integrand (Ri * scattering wave * bound state * potential * bound state * scattering wave * Rout) to include in the grid. If the integrand at a point (Ri,Rout,PHI) is smaller than DWCUTOFF times the largest value of the integrand encountered, that point will not be included in the grid. DWCUTOFF is used in both the construction of the grid and the computation of the radial integrals for each Li, Lout and Lx.

The lower and upper limits of the SUM grid are determined as the values of SUM for which the integrand has fallen (in a relative sense) beneath DWCUTOFF at DIF = PHI = 0. The scattering wavefunctions for L = LMIN are used when finding the lower limit of SUM while the wavefunctions for L = Lcritical are used for the upper limit. These two limits may be overriden by using the SUMMIN and/or SUMMAX keywords to give values (in fm) of the lower and upper limits.

The SUM grid points are mapped into the interval (SUMMIN, SUMMAX) in a manner that clusters them about a "midpoint." This midpoint is at present chosen to be the expectation value of SUM (weighted by the integrand for L = Lcritical) for DIF = PHI = 0. The value of the "midpoint" may be overridden with the keyword SUMMID or it may be multiplied by a factor specified by the MIDMUL keyword.

The form of mapping used for the SUM grid may be controlled by the MAPSUM keyword which may have one of the following values:

0 - linear mapping with no compression.
1 - cubic mapping with Sinh compression.
2 - rational mapping with Sinh compression (default).
3 - linear mapping with Sinh compression.

SUMMAP = 2 gives the best results in the cases so far examined and is the default. The degree of compression in mappings 1-3 is controlled by the GAMMASUM keyword. Suitable values are indicated in the table below.

The DIF grid limits are determined by the values of DIF for which the form factor becomes smaller in a relative sense than DWCUTOFF. These limits are chosen separately for each value of SUM. The DIF grid is also mapped about a "midpoint" which is chosen to be the location of the maximum of the form factor for the fixed value of SUM (and PHI = 0). Since the automatic choice of the DIF limits and midpoints seems always to be successful, no keywords are provided to override these values. The keyword MAPDIF is used to choose the DIF mapping and has the same meanings as the MAPSUM keyword. The best value in the cases studied is 1 which is the default. The keyword GAMMADIF specifies the degree of compression used in the mapping.

The PHI maps are individually chosen for each value of SUM and DIF. The minimum PHI is always 0 and the maximum is determined as the point at which the form factor falls in a relative sense beneath DWCUTOFF. For heavy ion reactions this is usually a small angle [Cos(PHI) > .99]. The PHI map is a linear map in the variable Cos(PHI).

Since the same three-dimensional grid is used for all values of Li, Lout, and Lx, there will be values of Ri and Rout for some Li, Lout, and Lx such that there is no significant contribution to the radial integral. For this reason the product of the distorted waves and a representative form-factor product is compared (in a relative sense) to DWCUTOFF for each (Ri, Rout) pair. If this product is less than DWCUTOFF, the PHI integral for that (Ri, Rout) is skipped. This procedure typically results in the skipping of 25% of all (Li, Lout, Lx, Ri and Rout) possibilities and since most of the skipped values occur for large Li and Lout (due to the centrifigal barrier), the time saved is proportionately greater.

The computation of the two-body wavefunctions (both bound and scattering states) may be controlled with the ASYMPTOPIA and STEPSIZE or STEPSPER keywords. ASYMPTOPIA specifies (in fm) the radius at which the wavefunctions are to be assumed to be asymptotic. For the bound states it is the largest value of Rp or Rt at which the wave functions will be found and thus must be large enough to satisfy the needs of the integration grid. The largest values of Rp and Rt used by the integration grid are printed in the summary of the grid. If the bound state ASYMPTOPIA prove to be limiting factors in the grid construction, a warning message will be printed indicating that ASYMPTOPIA should be increased in future runs. The increased value should be at least 5 fm larger than the values printed in the warning message. The calculation should be

repeated with this increased value since the radial integrals computed with the smaller grid may not be accurate. The largest value of Ri and Rout (the scattering variables) will automatically be chosen to be large enough to satisfy the needs of the integration grid. However it will never be smaller than the value of ASYMPTOPIA in effect at the time of input of the optical potentials.

The keyword STEPSIZE gives the increment used in the solution of the bound and scattering -state Schroedinger equations. Since arrays must be constructed that have ASYMPTOPIA/STEPSIZE elements, one should avoid making this ratio very large. The keyword STEPSPER may be used to specify the number of steps to use per wavelength. If it is entered, STEPSIZE will be computed according to the formulas:

STEPSIZE = Min(1/kappa, A) / STEPSPER : Bound states
STEPSIZE = Min(lambda, 2*A) / STEPSPER : Scattering

where "kappa" is the bound state inverse range:

kappa = sqrt(2*M*|E|) ,

and "lambda" is the scattering wavelength:

lambda = 2*Pi / sqrt(2*M*E) .

In both cases "A" is the diffuseness of the real part of the central Woods-Saxon well. It is suggested that STEPSPER be used instead of STEPSIZE since then the step size will automatically be adjusted as the wavelength changes due to changes in the scattering energy. If both STEPSIZE and STEPSPER are defined, STEPSPER has precedence. ASYMPTOPIA and STEPSIZE or STEPSPER may be respecified for each of the four two-particle states; if they are not reentered, the value last entered is used.

The keyword PARAMETERSET may be used to select standard groups of grid setting parameters. The keyword is followed by the name of one of the groups and will cause the grid setting parameters to be set as indicated in Table I. Individual settings may then be overridden by subsequently entering the appropriate keywords. Since the PARAMETERSET groups of Table I define values of ASYMPTOPIA and STEPSPER that are to be used in the two-body states, the PARAMETERSET keyword should precede the definitions of the two-body states. The line labeled "Accuracy" in Table I gives the percent error in the maximum cross section. The CA60A and CA60B PARAMETERSET names are appropriate for 160 on Ca calculations near 60 MeV. The PB100A, PB100B, and PB100C PARAMETERSET names are designed for 160 on Pb reactions near the Coulomb barrier. Note that STEPSPER and not STEPSIZE is defined by these PARAMETERSET sets. Since STEPSPER has precedence over STEPSIZE, one must use the command

UNDEFINE STEPSPER, STEPSIZE = ssss

if one wants to enter a specific STEPSIZE after having used PARAMETERSET (UNDEFINE is defined in Sec. VIII).

Table I shows that as one increases the numbers of grid points, one should also reduce DWCUTOFF so as to include more of the integrand in the computation. This reduction in turn means that ASYMPTOPIA may have to be made larger. The larger intervals that result from the smaller DWCUTOFF will also result in the Gauss points being spread out further so that the same number of points

TABLE I

PARAMETERSET names and associated values. The first column gives the default values.

Keyword	Default	CA60A	CA60B	PB100A	PB100B	PB100C
LSTEP	1	3	2	5	4	3
DWCUTOFF	10^{-3}	10^{-2}	10^{-3}	$3*10^{-3}$	10^{-3}	10^{-4}
NPSUM	32	24	32	24	32	48
NPDIF	10	10	13	10	11	12
NPPHI	10	10	12	10	12	14
LMINMULT	.6	.6	.5	.86	.78	.70
LMAXADD	30	15	20	20	25	30
GAMMASUM	5.	5.	5.	2.	2.	2.
GAMMADIF	5.	5.	5.	3.	3.	3.
ASYMPTOPIA	20.	20.	25.	30.	35.	40.
STEPSIZE	.1	none	none	none	none	none
STEPSPER	none	15	40	8	12	20
Accuracy		0.7%	0.1%	1.5%	1.%	?

will give reduced accuracy.

It is suggested that for each substantially new problem, the user make calculations with several different sets of grid parameters to verify that convergence has been achieved.

VI - Stand-Alone Two-Body Calculations

One may use the facilities of Ptolemy to compute the properties of two-body bound or scattering states without doing a complete DWBA calculation. Such calculations will be referred to as "stand-alone" two-body calculations. They are done by defining the two particles and the potential that acts between them and then entering a semicolon to start the calculation. If the energy is negative a bound state calculation will be made, if it is positive the two-body scattering will be computed. If desired one may use the keywords BOUNDSTATE or SCATTERING to indicate which is to be done and the energy will be checked for validity. Although it is possible to mix stand-alone and DWBA calculations in one job, it is recommended that separate jobs be used for stand-alone and complete DWBA runs. However many stand-alone calculations of both bound states and scattering may be done in one job.

The two particles involved in the stand-alone calculation are referred to as the "projectile" and "target." These words have their customary meanings for scattering states; the only distinction for bound states is that the projectile's angular momentum is used to determine the spin-orbit force.

The CHANNEL keyword may be used to specify the nuclei in the channel. Some examples will illustrate its form:

```
CHANNEL  16O + 208PB
CHANNEL:  P + 15N = 016
CHANNEL =  209BI(7/2- .9) = P + 208PB
```

The first example gives a scattering state while the other two define bound states. Note that in the case of bound state channels, the resultant bound state may be either the first nucleus (inwhich case it is followed by an equal sign) or the last nucleus. The syntax of the nucleide specifications is the same as for the REACTION keyword (page 26). Any or all of the two or three nuclei may be given an excited state specification which also has the same syntax as for the REACTION keyword. In all cases the projectile and target must be separated by a plus sign and <u>the projectile always comes first</u>. If a bound state is being specified, the composite nucleus may be either first or last and must be separated from the other two nuclei by an equal sign. The CHANNEL keyword and the complete channel specification must be contained on a single input line. The CHANNEL keyword will define the projectile and target mass, charge, and intrinsic spin. In addition for bound states the total angular momentum and the bound state (cluster separation) energy are also defined.

If the CHANNEL keyword is not used, the particle masses may be entered with the keywords MP and MT which give the masses in AMU of the projectile and target respectively. Alternatively one can use the keyword "M" to enter the reduced mass in MeV/c^2. The charges of the two particles may be entered with the keywords ZP and ZT. The projectile and target intrinsic spins may be entered with the keywords SP and ST. The total angular momentum of a bound state may be entered with the keyword "J." It is not necessary to enter J or ST (the calculation does not depend on them) and SP is necessary only if there is a spin-orbit force.

The potential parameters are entered with the keywords defined in Sec. IV-B (page 29). The number of nodes in the bound state wavefunction and its orbital angular momentum are defined by the keywords NODES and L. If a spin-orbit force is present in the bound state, it is also necessary to define JP. The NODES, L, and JP keywords are discussed more fully in Sec. IV-B. The keywords FITE and FITV which are defined in Sec. IV-B may be used in bound state calculations.

The c.m. energy may be entered using either of the keywords ECM or E. In the case of bound states one of these should be used to enter the energy as a negative number unless the CHANNEL keyword is used. The laboratory scattering energy may be entered with the keyword ELAB. In this case both MP and MT must be defined to allow the conversion to the c.m. energy.

If a scattering calculation is being made, one may indicate either a range of orbital angular momentum values by using the LMIN and LMAX or the LMINMULT and LMAXADD keywords or one may specify a single value of the orbital angular momentum by using the keyword "L". If a spin-orbit force is entered for a scattering problem, the S-matrices will be computed for all values of Jp connected with each value of L (note that Sp is not limited to 1/2 for spin-orbit forces). If it is desired to have only one value of Jp, the keyword JP may be used to specify that value. If both of the keywords "L" and "JP" are used, only one scattering partial wave will be computed.

The keyword ELASTIC may be used to cause the elastic differential cross sections to be computed. In this case the ANGLEMIN, ANGLEMAX and ANGLESTEP keywords (page 33) will determine the angular grid to be used. The default is NOELASTIC which suppresses the differential cross sections. One should note that the extrapolation to large L-values that is provided in DWBA calculations does not occur in elastic scattering calculations. Thus a larger LMAX or LMAXADD is required for elastic scattering calculations.

The computed wave functions (for both bound and scattering states) will be printed if the keyword WRITESTEP is used. This keyword specifies the stepsize for which the wavefunction is to be tabulated. The value of WRITESTEP should be a multiple of STEPSIZE (page 35) ; if it is not, the closest multiple of STEPSIZE will be used. Setting WRITESTEP equal to 0 (the default) will suppress the printing of the wavefunction.

The bound state wavefunctions are the solutions of the Schroedinger equation

$$\{ \hbar^2/(2Mr^2) [-(d/dr) r^2 (d/dr) + L(L+1)] + V(r) - E \} Phi(r) = 0 ,$$

while the scattering wavefuncitons are the solutions of

$$\{ \hbar^2/(2M) [-d^2/dr^2 + L(L+1)/r^2] + V(r) - E \} f(L)(r) = 0 .$$

The bound state wavefunctions are normalized to unity so that

$$\text{Integral}(0 \text{ to infinity})\ dr\ r^2\ Phi^2 = 1$$

The scattering wavefunctions are normalized to have the asymptotic form

$$f(r) \longrightarrow (1/2) * \{ (1+S)*F(kr) + i\ (1-S)*G(kr) \}$$

where F and G are the regular and irregular Coulomb functions.

Note that asymptotically the bound state wave functions behave as exp(-kappa*r)/r while the scattering wavefunctions have the asymptotic behavior exp(ikr).

The name of the bound state wavefunction will be PHIn where "n" is an integer that is 1 for the first bound state and is increased by 1 for each subsequent bound state. After n = 9, it is set back to 1 again. Thus one can have up to nine bound state wavefunctions in the allocator at once. The names of the real and imaginary scattering wave functions will be WAVER and WAVEI. If it is desired to have more than one scattering wavefunction in the allocator at once, the keywords RENAME or COPY should be used (see Sec. VIII).

Normally only the last computed scattering wavefunction will be available if a range of L's or Jp's is specified. The keyword SAVEWAVE will cause each scattering wavefunction to be saved in a separate unnamed object in the allocator. The keyword NOSAVEWAVE may be used to stop the effects of SAVEWAVE; NOSAVEWAVE is the default.

The keyword CHECKASYMPT may be used to show the rate of convergence of the scattering wavefunctions to the asymptotic form given above. The difference of the exact wavefunction and the asymptotic form will be printed at intervals determined by WRITESTEP (which must also be defined). The keyword NOCHECKASYM cancels a previously entered CHECKASYMPT and is the default.

VII - Optical Model Potential Fits

Ptolemy provides a powerful and efficient program for fitting optical model potentials to elastic scattering data. Optical model fits are usually made as stand-alone calculations but it is possible to include them in the same job as DWBA calculations. The input for an optical model fit consists of the following items:

1) specification of the scattering channel,
2) specification of the potential parameters that are to be varied in the fit,
3) initial values of the search parameters and the fixed values of all other potential parameters,
4) experimental data,
5) parameters to control the fit and elastic scattering calculations.

Items 1 to 5 may be given in any order. The end of the input for a fit is signaled by a semicolon (;) which causes the fit to begin. When the fit is complete, the potential parameters will be set to the best potential parameters that were found. In addition the predicted optical model scattering cross sections will be printed for each experimental point that was included in the fit. The user may then enter control lines to compute the elastic scattering on a uniform angular grid, or he may increase the accuracy of the calculation (through the use of keywords such as LMINMULT, LMAXADD, STEPSPER or FITACCURACY) and resume the search by entering a second semicolon.

The specification of the scattering channel and of the potential parameters is made using the keywords introduced in Sections IV-B and V. Both the fixed and initial potential parameters are entered using the potential keywords of section IV-B. The LMIN, LMAX, LMINMULT, LMAXADD, STEPSIZE, STEPSPER and ASYMPTOPIA keywords (pages 32 and 35) may be used to control the accuracy of the elastic scattering calculations during the search.

The parameters to be varied in the fit are specified by the FIT keyword. This keyword is followed by a list of potential parameters (page 29) to be varied. The list must be enclosed in parentheses. If two or more potential parameters are to be held equal to each other during the fit, they should be joined by an equal sign in the FIT list. Some examples of valid FIT specifications are:

```
FIT ( V VI )  - a two-parameter fit;
FIT ( A=AI, AE=AIE, V )  - a three-parameter fit with
    the same energy dependance in A and AI;
FIT ( R0=RI0=RC0 )  - a one-parameter fit.
```

Each FIT parameter must have its initial value explicitly entered by means of the potential-defining keywords of Sec. IV-B. The initial value of the first of a string of equal parameters is the one that will be used to start the search.

The experimental data are entered using the DATA keyword. This keyword is followed by a pair of parentheses that enclose all of the data that are to be used. If a second DATA keyword occurs in a given job, it will replace, not supplement, the data entered

with the first keyword. The data are entered in one or more groups, each containing data at a single laboratory energy. Each group is preceded by a list of keywords that give the laboratory energy, optional overall weight and renormalization factors, and the type of data to be entered. The laboratory energy of the group of data is specified using the ELAB keyword and is in MeV. Each data item is weighted in the chi-squared sum by the square of the inverse of its experimental error. An overall weight factor that will multiply each of these individual weights may be entered using the WEIGHT keyword. The keyword RENORMALIZATION may be used to enter a renormalization factor that is multiplied into each experimental value before computing the chi-squared sum. If WEIGHT or RENORMALIZATION are not entered, the default value of unity is used.

The laboratory angles of the data can be shifted by a constant angle with the ANGLESHIFT keyword. This keyword specifies an increment (in degrees) that is to be added to each angle in the laboratory frame. The input c.m. angles and data are transformed to the laboratory frame for this shift. After the shift, the Jacobian relating the c.m. and laboratory frames is recomputed at the new angle, and the angles and data are transformed back to the c.m. frame. Furthermore if the cross sections are given as ratios to the Rutherford cross sections, the data values are changed to correspond to the Rutherford cross sections at the new angles. Thus this keyword treats the data as if the absolute normalization of the data is experimentally known. If the data was normalized to the Rutherford cross section for small angles, it will be necessary to use the RENORMALIZATION keyword to specify a suitable renormalization factor [the average (over the small angles) of the ratios of the Rutherford cross sections at the original and shifted angles] for the shifted data.

The type of data that is being entered is indicated by the SIGMA or SIGMATORUTH keywords which respectively mean that the data values are cross sections in millibarns or ratios of cross sections to the Rutherford cross section. The keywords MBERROR or PERCENTERROR are used to indicate that the experimental errors are being entered in mb or as a percentage of the experimental values. The ANGLE keyword is used to designate center-of-mass angles in degrees (at present this is the only choice). The order of these keywords (SIGMA or SIGMATORUTH, MBERROR or PERCENTERROR, and ANGLE) is used to specify the order of the data that follows. The keywords are followed by triples of numeric values that give the data in the order of the keywords. These triples are terminated by either more keywords (which would be used to introduce data at a different energy or with a different overall weight or renormalization) or by the closing parenthesis. As many cards as are necessary may be used to enter the data; the end of the DATA keyword is signalled by the closing paranthesis.

The following example illustrates the DATA keyword:

```
DATA ( ELAB=48  ANGLE PERCENTERROR SIGMATORUTH
  10 5 1.023,  12.5 2 .99   20 3.3 .5
  30  15  .12
  ELAB = 56   WEIGHT = .5   ANGLE SIGMA MBERROR
  10  3.  .3,   15 1. .1  20 .1 .1   )
```

Here we are entering data at two different energies. The data at the first energy is given at angles of 10, 12.5, 20, and 30 degrees and consists of ratios to the Rutherford cross section that are respectively 1.023, .99, .5, and .12. The errors in these numbers are given as percentages. The data for the second energy are given in millibarns with errors also specified in millibarns. If data that consists of the same quantities in the same order is to be entered at several energies, it is not necessary to repeat the ANGLE, SIGMA or SIGMATORUTH, and MBERROR or PERCENTERROR keywords for each energy.

One of the keywords LMCHOL, QUAVER, MINIM, DAVIDON, POWELL65, OCOPTR, ROCORD or LMGENV may be used to pick the minimizing program that is to make the search. The average user will have need of only the default which is LMCHOL. The keywords FITMODE, FITMULTIPLE, FITRATIO, NUMRANDOM, and REINITIALIZE are used by some of the following fitters; the default values will almost always suffice. A description of these minimizers follows:

1) LMCHOL - This is a minimizer that uses analytically computed gradients and makes specific use of the sum-of-squares property of the function that is being minimized. The analytic gradients are computed as the expectation value in the distorted waves of the derivatives of the potential. The potential derivatives are evalued numerically. LMCHOL is based on the HARWELL subroutine VA07A which was coded by Fletcher. Despite the fact that the computation of the gradients can more than double the chi-squared sum evaluation time, the LMCHOL and QUAVER fitters usually find a minimum in less than half the CPU time required by the other fitters. We know of no cases inwhich the CPU time is significantly longer for LMCHOL. The LMCHOL fitter is therefore highly recommended and is the default fitter.

2) QUAVER - This is a quasi-Newton fitter that uses a pseudo-inverse procedure to solve the required systems of linear equations. The keyword FITRATIO may be used to eliminate steps alcng poorly determined linear combinations of the optical model parameters. The default value of 10^{-4} will have this effect; smaller values (such as 10^{-15}) will eliminate such restrictions on the search direction. For most fits QUAVER is almost identical to LMCHOL in performance. Setting PRINT=2 (page 49) will cause the singular values (the quantities that indicate which linear combinations of parameters are poorly determined) to be printed at each iteration. For both the QUAVER and MINIM fitters, the keyword FITMULTIPLE is a divisor used to reduce the step length when a step to a larger function value is attempted. The default value is 5.

3) MINIM - This is a variable-metric fitter using the 1972 Fletcher presciption for the metric update. It is generally slower than the above two fitters.

4) DAVIDON - This uses the original variable-metric prescription of Davidon. It is based on the Davidon

fitter found in the Argonne Applied Mathematics Divison library. This fitter is somewhat slower than the Fletcher fitter (MINIM). The keyword FITMULTIPLE determines the initial estimate of the metric matrix. The default (FITMULTIPLE = 0 or FITMULTIPLE > 100) is to use the second derivative approximation generated from the Jacobian of the chi-squared function. If FITMULTIPLE is set to a nonzero value, a diagonal matrix will be used as the initial metric and thus the search will start along the gradient direction. The diagonal elements of the matrix will be |FITMULTIPLE|*D(i) where D(i) = 1 if FITMULTIPLE > 0, and D(i) = x(i)**2 if FITMULTIPLE < 0 (x designates the parameter vector). The keyword NUMRANDOM may be used to specify the number of random steps that are to be made in confirming a minimum. The default is zero.

5) POWELL65 - This is a minimizer that makes specific use of the sum-of-squares property of the function but does not require Ptolemy to evaluate the gradient of the function. It is the Harwell subroutine VA02A which is based on a 1965 paper of Powell. The POWELL65 search algorithm is usually quite efficient for the first few iterations but then often begins to take very small steps for subsequent iterations. Therefore it often pays to terminate the search intermittently and restart it again. This may be accomplished by using the keyword REINITIALIZE to specify the number of iterations between restarts. REINITIALIZE = 16 is a reasonable value for POWELL65; the default is zero which suppresses reinitialization. The keyword FITMULTIPLE is used to limit the size of a single step; no step will be allowed to exceed FITMULTIPLE*FITACCURACY in relative size. The default is 500, but some tests indicate that larger values (10000) may result in faster searches.

6) OCOPTR - This is a minimizer that does not make specific use of the sum-of-squares property of the function that is being minimized. Therefore it generally requires considerably more chi-squared evaluations than the preceding minimizers. However it is concievable that there will be circumstances in which the above minimizers will lose their way and OCOPTR is provided as an alternative for such cases. When using this fitter, FITMULTIPLE=3 should be specified.

7) ROCORD - This minimizer also does not make use of the sum-of-squares property of the function. It is also provided as an alternative should the preceding minimizers fail to behave reasonably. The keyword FITMODE may be used to specify the initial value of IRET for ROCORD; the default is -1021. The keyword NUMRANDOM has the same meaning as for the DAVIDON fitter.

8) LMGENV - This minimizer is similar to POWELL65 in that it makes use of the sum-of-squares property but does not require analytic gradients. It is also based on a Harwell routine (VA05A) written by Powell and is

apparently intended to replace the routine used by POWELL65 (VA02A). However it has proven to require considerably more function references than POWELL65 and hence is not at present recommended. It is hoped that this routine will eventually be improved so that it will replace POWELL65 in later versions of Ptolemy.

The FITACCURACY keyword may be used to specify the accuracy with which the potential parameters are to be found. Its significance depends upon which minimizer is used but for the first five fitters above it gives the relative accuracy to which each potential parameter or the minimum chi-squared value is to be found. The default value is 10^{-3}. The MAXFUNCTION keyword limits the number of chi-squared sums that may be evaluated during a search. Its default value is 50 which is more than enough for the default fitter (LMCHOL).

VIII - Control Keywords

In this section we describe some of the control keywords that are available in Ptolemy. These keywords may generally be placed anywhere in the Ptolemy input and they usually cause some sort of immediate action. These keywords are listed more or less in decreasing order of interest.

The HEADER keyword may be used to enter a header that will be printed on the top of most pages of the Ptolemy output. The header will consist of the remainder of the input line beginning with the first alphanumeric following the HEADER keyword. In addition the REACTION specification (if it is entered) and the laboratory energy will always be part of the header.

The SIZE keyword may be used to specify the size of the allocator (the Ptolemy work area). If the SIZE value is given as a positive number, it is the size in bytes of the allocator. It is usually more convenient to enter a negative number which is interpreted as the number of bytes of core to leave for other purposes (such as I/O buffers); the remainder of the available core is used for the allocator. The default value of SIZE is -5000. This default is generally adequate but may be made closer to zero if no KEEP operations are anticipated.

The RETURN keyword should be used as the last keyword in every Ptolemy job. It causes allocator statistics to be printed and then returns control to the operating system.

The KEEP keyword is used to keep Ptolemy results in a form suitable for later recovery with the Speakeasy KEPT command. A Speakeasy KEEP dataset must be allocated to the file (DD name) MYKEEP if the KEEP keyword is to be used. Appendix C shows the JCL required to make such a dataset and to include it in the Ptolemy job. KEEP must be followed by two names: the first is the Ptolemy name of the item to be kept; and the second is the name under which it is to be saved in the dataset. This second name must be different from all other names already in the dataset or else the new object will replace the previously-kept object. The following is a list of the Ptolemy names of the objects the user is most likely to want to keep:

CROSSSEC - The differential cross section on the (ANGLEMIN, ANGLESTEP, ANGLEMAX) grid. For DWBA calculations this contains the reaction cross section. For stand-alone elastic scattering it contains the elastic differential cross sections. In both cases it is in mb/sr.

TORUTHERFORD - The ratio of the elastic scattering differential cross section to the Rutherford cross section. This array is produced only in stand-alone elastic scattering.

IMAG - The magnitude of the radial integrals.

IPHASE - The phase of the radial integrals.

In the above two objects, the element corresponding

to a given Li, Lout, Lx is found by using the subscript

$$I = (Lout-LMIN)*Num(Li,Lx) + \{ (Lx+Lxmin+1)*(Lx-Lxmin) + Li+Lx-Lout \}/2 + 1$$

where

Lxmin is the minimum Lx appearing in the calculation,

Lxmax is the maximum Lx, and

Num(Li,Lx) is the maximum number of (Li,Lx) combinations one can have for a given Lout:

$$Num(Li,Lx) = \{ (Lxmax+Lxmin+2)*(Lxmax-Lxmin+1) \}/2$$

(This expression does not take into account abnormal parity restrictions but it is always the correct expression to use for computing the subscript I).

SIN - The elastic S-matrix elements in the incoming channel.

SOUT - The elastic S-matrix elements in the outgoing channel.

The SAVEHS keyword is used to initiate the saving of the integrals over PHI of the form factor. These integrals may then be reused in later calculations with different optical potentials at a considerable saving in CPU time. The SAVEHS keyword must be entered before the first semi-colon and should be entered after the HEADER and REACTION keywords if they are used. If SAVEHS is used the Fortran file (DD name) FT01F001 must be defined (see Appendix C).

The USEHS keyword is used to indicate that the H-integrals saved in a previous calculation with the SAVEHS keyword are to be reused. USEHS must be entered before the first semicolon. If it is used, the REACTION, LSTEP and all grid-setting keywords should not be used. The bound state potentials must not be entered; rather the definitions of the new optical potentials should directly follow the USEHS keyword. These definitions are then followed by the final semicolon indicating that the DWBA calculation is to begin. If ELAB, LMIN, and/or LMAX are not specified, the SAVEHS values will be used. However new values of these parameters may be specified in the USEHS run. If a different LMIN is specified, the user must insure that it was one of the values explicitly computed in the SAVEHS run (i.e. that LMIN = LMIN(SAVEHS) + n*LSTEP). If a new value of ELAB is specified, the SUM grid will not be the optimal grid since it was chosen for a different energy. In cases inwhich it is desired to do USEHS runs at different energies, the SAVEHS run should be made at the maximum energy to be used. It should be made with more SUM points than would be necessary for a calculation at a single energy and should be made with a small value of GAMMASUM (say GAMMASUM = 1). This "detuning" of the SUM grid results in a grid adequate for more than one energy.

The KEYWORDS keyword may be used at any time to cause a listing of the current settings of all data-entering and option-choosing keywords. It is suggested that it be used at the end of all runs to provide a verification of the parameters and options in effect. The LISTKEYS keyword will list the names of all valid keywords. It is useful in TSO applications to check the

spelling of a keyword.

The UNDEFINE keyword may be used to set the status of a keyword to "undefined." It is followed by the name of the keyword that is to be undefined. The most likely use of UNDEFINE is to undefine a potential radius (R, RI, etc.) during stand-alone calculations so that it will automatically be computed from the corresponding radius parameter (R0, RI0, etc.) the next time it is needed.

The NSCATALOG keyword may be used at any time to provide a list of the names and sizes of all currently defined objects in the allocator. It will also give the NSSTATUS output.

The NSSTATUS keyword will cause a short summary of the allocator status to be printed. This summary will show the allocator size, its current in-use size and the peak in-use size. This summary is automatically printed at the end of all Ptolemy jobs.

The DUMP or NSDUMP keywords may be used to print an object in the allocator. They are followed by the name or number of the object to be printed.

The RESET keyword may be used to cause Ptolemy to be set back to its initial status. The complete allocator is cleared and all keywords are set to their default values. However the allocator size may not be changed after a RESET. The use of RESET allows several independent calculations to be made in one job. If it is desired to do a SAVEHS calculation and immediately follow it with several USEHS calculations, each USEHS step should be preceded with a RESET.

The CLEAR keyword causes the allocator to be cleared. All objects are removed from the allocator. However none of the keyword settings are changed. The size of the allocator may not be respecified after a CLEAR command.

The COPY keyword may be used to copy the data in an object in the allocator into a second object. The form of the command is

COPY fromname toname

where "fromname" must be the name of an object already in the allocator. If "toname" already exists in the allocator and is the same size as "fromname," the data in "fromname" will be copied into "toname." Otherwise "toname" will be created (or changed to have the correct size) and then the copy will occur. In all cases "fromname" is not changed. The COPY command may be used to "fool" Ptolemy into using a different potential or wavefunction in a subsequent part of the calculation.

The RENAME command is used to change the name of an object in the allocator. Its form is

RENAME oldname newname

where "oldname" must be the name of an object in the allocator. The name of this object will be changed to "newname." There must not be another object with the name "newname" already in the allocator; if there is, inconsistent results may occur.

The FREE command is used to delete an object from the

allocator and thus make its space available for other objects. The command is followed by the name of the object to be freed. If the object does not exist, a warning will be printed and processing will continue with the next input line.

In the COPY, RENAME and FREE commands the first object name may be replaced with the actual number of the object in the allocator. However this practice is not recommended since it is difficult to predict the numbers of the objects.

The BIMULT keyword causes two objects (they may be the same object) to be multiplied together. The form of the command is

BIMULT name1 name2

where "name1" and "name2" are the names of the two arrays to be multiplied together. They must be of the same length. They will be multipied together in an element-by-element fashion and the resulting array will be stored in a new unnamed object in the allocator. Its number will be printed in the output. The numbers of the input arrays may be used inplace of their names.

The keyword NUMRNUM may be used to compute the matrix element between two wavefunctions of a power of r. The form of the command is

NUMRNUM name1 power name2

where "name1" and "name2" are the names (or numbers) of two objects in the allocator. They must be of the same length and must be wavefunctions that were computed with the present value of STEPSIZE. The integer "power" is the power of r that is to be included in the integral. The integral

Integral(0 to ASYMPTOPIA) dr r**power name1 name2

will be computed and printed.

The keyword NRNLIMS may be used to compute the partial matrix element of a power of r. The form of the command is

NRNLIMS name1 power name2 start stop

where "name1", "name2," and "power" are the same as for NUMRNUM. The range of the integral is specified by "start" and "stop" which are specified in fm.

The keyword PRINT may be used to control the amount of printing that Ptolemy does. It is followed by a four-digit integer that indicates the amount of printing that is to occur. Each digit controls different items of the printed output. The larger the digit, the more information that is printed. The default value is PRINT = 0001 (the leading 0's are not necessary) which results in summaries of the input, the radial integral phases and magnitudes and the cross sections being printed. If the four-digit number is writen as PRINT = MCXI, the significance of the digits is:

I = 0 - Only print the differential cross sections and final fit values.

1 - (Default) - Print summaries of input, magnitudes and phases of the radial integrals and elastic S-matrices in addition to output for PRINT=0. For fits the initial and final values are shown along with a summary of the path followed

by the fitter.
2 - Print radial integrals as they are computed and give estimates of their cancellations; show convergence to the bound state potential or energy; print elastic S-matrices as they are computed. The singular values are printed by the QUAVER fitter.
≥ 3 - Print debugging information.

X = 1 - The WKB amplitudes used to find the critical L are printed for each L.
2 - Much debugging output is printed by the WKB routine (beware!).

C = 1 - Several lines are printed for every chi-squared function calculation made during the course of a fit.

M = 1 - The elastic S-matrix element is printed every time a scattering wavefunction is computed.
4 - Debugging output is produced by the elastic wavefunction routine.

The value of PRINT may be changed at any time to effect subsequent printing except that the value of PRINT that was in effect at the time of the specification of the outgoing scattering state will determine the printing of the elastic S-matrices during the computation of the radial integrals.

IX - Acknowledgements

We wish to thank Frank Serduke for making available the subroutines that supply the data on nuclear charges, mass excesses, and spins. Larry Nazareth has been most helpful in giving us advance access to a number of subroutines that are being considered for inclusion in the Argonne Applied Mathematics Division MINPACK project.

Appendix A - List of all Keywords

The following lists contain brief descriptions and default values for all the Ptolemy keywords. Some of these keywords have not been discussed in the above text either because they are primarily designed for use in debugging Ptolemy or because it is doubtful that the average user will need them. They are all included here for completness.

The entry "none" under "Default" means that the keyword is initially undefined. If it is not defined in the input and is necessary to the calculation, an error message will be printed and the job aborted. The entry "none*" under "Default" means that the keyword is initially undefined, but if it is not defined in the input, an appropriate value will be found by Ptolemy.

The keywords CROSSSECTION, GRIDSETUP, LINTERPOL, and RADIALINT are used inplace of the final semicolon to initiate individual stages of the DWBA calculation and should not be used in standard calculations. If desired the keywords DWBA or NZRDWBA may be used before the final semicolon to indicate that a DWBA calculation is to be done but they are not, at present, necessary.

All lengths are specified in fm and all energies are in MeV.

Reaction-defining keywords

Keyword	Default	Meaning
E*i	0	Excitation energy in MeV of nucleus i (i = A, B, BIGA, BIGB, or X)
ECM	none	Incoming c.m. scattering energy in MeV
ELAB	none	Incoming Laboratory scattering energy in MeV
Ji	none	Intrinsic spin of nucleus i (i = A, B, BIGA, BIGB, or X)
Mi	none	Mass in AMU of nucleus i (i = A, B, BIGA, BIGB, or X)
MXCi	none	Total mass excess in MeV of nucleus i (i = A, B, BIGA, BIGB, or X)
MXCGi	none	Ground state mass excess in MeV of nucleus i (i = A, B, BIGA, BIGB, or X)
Q	none	Q-value in MeV
REACTION	none	Defines reaction in standard notation
SPAMP	1.	Projectile spectroscopic amplitude
SPAMT	1.	Target spectroscopic amplitude
SPFACP	1.	Projectile spectroscopic factor
SPFACT	1.	Target spectroscopic factor
Zi	none	Charge of nucleus i (i = A, B, BIGA, BIGB, or X)

Two-body state keywords

Keyword	Default	Meaning
A	none	Real W.S. diffuseness
AE	0	AE*Elab is added to A
AESQ	0	AFSQ*Elab² is added to A
AI	none	Imaginary W.S. diffuseness
AIE	0	AIE*Elab is added to AI
AIESQ	0	AIESQ*Elab² is added to AI
ASI	none	Surface absorption diffuseness
ASO	none	Real spin-orbit diffuseness
ASOI	none	Imaginary spin orbit diffuseness
CHANNEL	none	Specifies a two-body channel.
E	none	Two-body c.m. energy in MeV
J	none	Total two-body angular momentum
JP	none	Total projectile ang. mom. (for spin-orbit)
L	none	orbital angular momentum
M	none	Reduced mass in MeV/c**2
MP	none	Projectile mass in AMU
MT	none	Target mass in AMU
NODES	none	Number of bound state nodes for r > 0
R	none	Real W.S. radius
R0	none	Real W.S. radius parameter
R0E	0	R0E*Elab is added to R0
R0ESQ	0	R0ESQ*Elab² is added to R0
RC	none	Coulomb radius
RC0	none	Coulomb radius parameter
RI	none	Imaginary W.S. radius
RI0	none	Imaginary W.S. radius parameter
RI0E	0	RI0E*Elab is added to RI0
RI0ESQ	0	RI0ESQ*Elab² is added to RI0
RSI	none	Surface absorption radius
RSI0	none	Surface absorption radius parameter
RSO	none	Real spin-orbit radius
RSO0	none	Real spin-orbit radius parameter
RSOI	none	Imaginary spin-orbit radius
RSOI0	none	Imaginary spin-orbit radius parameter
SP	none	Projectile spin
SPAM	none	Channel spectroscopic amplitude
ST	none	Target spin
TAU	0	Real S.O. depth relative to real W.S. depth
TAUI	0	Imag S.O. depth relative to imag W.S. depth
V	0	Real W.S. well depth
VE	0	VE*Elab is added to V
VESQ	0	VESQ*Elab² is added to V
VI	0	Imaginary W.S. well depth
VIE	0	VIE*Elab is added to VI
VIESQ	0	VIESQ*Elab² is added to VI
VSI	0	Surface absorption strength
VSO	0	Real S.O. well depth
VSOI	0	Imaginary S.O. well depth
ZP	none	Projectile charge
ZT	none	Target charge

Calculation keywords

Keyword	Default	Meaning
ACCURACY	10^{-12}	Accuracy of bound state convergence
ANGLEMAX	90	Maximum scattering angle in degrees
ANGLEMIN	0	Minimum scattering angle in degrees
ANGLESTEP	1	Scattering angle increment in degrees
ASYMPTOPIA	20	Start of asymptotic region
DATA	-	Enters experimental data for a fit
DELTAVK	.05	Bound state search step size
DERIVSTEP	10^{-6}	Stepsize for numeric gradient of potentials
DWCUTOFF	10^{-3}	Minimum relative integrand to use in DWBA integral
FITACCURACY	10^{-3}	Required relative accuracy of optical model parameter fit
GAMMADIF	5	DIF compression parameter
GAMMASUM	5	SUM compression parameter
LBACK	none*	LMAX-LBACK is start of L-extrapolation
LMAX	none*	Maximum scattering partial wave L
LMAXADD	30	LMAX = LMAXADD + Lcritical
LMIN	none*	Minimum scattering partial wave L
LMINMULT	0.6	LMIN = LMINMULT*Lcritical
LOOKSTEP	250	Number of steps in grid-searching for PHI
LSTEP	1	Increment of L in radial integral computations In-between values are found by interpolation.
LX	none	Exchanged orbital angular momentum
MAPDIF	1	Gauss-point map type for DIF grid
MAPSUM	2	Gauss-point map type for SUM grid
MAXFUNCTIONS	50	Maximum number of chi. sqr. computations allowed in an optical model fit
MAXITER	10	Max. number of iterations in bound state search
MAXLEXTRAP	100	Maximum allowed L-extrapolation
MIDMULT	1	SUMMID multiplier
NAITKEN	4	degree of interpolation polynomial
NBACK	4	Num. of backward steps in scattering wave asymptotic matching
NCOSINE	256	Size of fast-cosine table
NPDIF	10	Num. of points in DIF grid
NPHIADD	4	Num. of steps to extend PHI grid
NPPHI	10	Num. of points in PHI grid
NPSUM	32	Num. of points in SUM grid
STEPSIZE	.1	Step size for solutions of two-body differential equations
STEPSPER	none	Number of steps per "wavelength" for solutions of two-body equations.
STEP1R	1	Starting value for scattering state dif. eqn.

---

* A value will be computed by the program if one is not given by the user.

Calculation keywords

Keyword	Default	Meaning
STEP1I	1	Starting value for scattering state dif. eqn.
SUMMAX	none*	End of SUM grid
SUMMID	none*	Clustering point of SUM grid
SUMMIN	none*	Beginning of SUM grid

---

* A value will be computed by the program if one is not given by the user.

Control and option-selecting keywords

Keyword	Default	Meaning
ALLOCATE	-	Enter data into the allocator
BATCH	none*	Enter batch mode - an error terminates things
BIMULT	-	Multiply two arrays together
BOUNDSTATE	off	Stand-alone bound state is being entered
CHECKASYMP	off	Check approach of scattering state to asymptotic form
CLEAR	-	Clear allocator of all defined objects
COPY	-	Copy one object in the allocator into another
CROSSSECTION	off	Entering data for DWBA cross section stage
DAVIDON	off	Use the Davidon variable-metric fitter
DERIVCHECK	off	Check the analytic chi. sqr. gradients
DOASYMPT	on	Use Whittaker bound state asymptotic form
DOTSO	-	Enter the TSO Command mode
DUMP	-	Print an object in the allocator
DUMPALL	-	The entire allocator is printed
DUMP2	-	Print an integer*2 object in the allocator
DWBA	-	DWBA input is being entered
ECHO	on	Input lines are printed in the output
ELASTIC	off	Compute cross section in stand-alone scattering
FIT	off	Do an optical model fit and specify the parameters to be varied
FITE	off	The bound state energy is matched to the potential
FITMODE	1	Meaning depends on optical model fitter in use
FITMULTIPLE	500	Meaning depends on optical model fitter in use
FITRATIO	10^{-4}	Meaning depends on optical model fitter in use
FITV	on	The depth of the real part of the W.S. well is matched to the bound state energy
FREE	-	Remove an object from the allocator
GRIDSETUP	off	Grid setup input is being entered
HEADER	-	Defines the header for subsequent pages
INCOMING	off	The incoming scattering state is being defined
KEEP	-	Keep an object for subsequent Speakeasy use
KEYWORDS	-	List all keywords and their present values
KORFRE	-	Show size of unused core
LINEAR	off	Only use linear extrapolation in the bound state search
LINTERPOL	off	Input is for L-interpolation stage
LISTKEYS	-	List all keywords
LMCHOL	on	Use the LMCHOL sum-of-squares minimizer with
LMGENV	off	Use the LMGENV sum-of-squares minimizer
MINIM	off	Use the Fletcher variable-metric fitter
NOCHECKASYM	on	Do not check asymptotic form of scattering solution
NOECHO	off	Do not print input lines in the output

---

* A value will be computed by the program if one is not given by the user.

Control and option-selecting keywords

Keyword	Default	Meaning
NOELASTIC	on	Do not compute cross sections in stand-alone scattering problems
NOSAVEWAVE	on	Do not save elastic wavefunctions in the allocator
NRNLIMS	-	Compute partial overlap of two functions
NSCATALOG	-	List names of all objects in allocator
NSDUMP	-	Print an object in the allocator
NSSTATUS	-	Print allocator statistics
NUCONLY	off	Use only the nuclear part of the B.S. potential in the interaction potential
NUMRNUM	-	Compute overlap of two functions
NZRDWBA	off	Input is for a nonzero-range DWBA
OCOPTR	off	Use the OCOPTR generalized minimizer
OUTGOING	off	Input is for the outgoing scattering state
PARAMETERSET	none	Specify a group of keyword definitions
POWELL65	off	Use the Powell 1965 sum-of-squares minimizer
PRINT	1	Controls amount of printing
PRINTFIT	-	Print present E and V
PRINTWAV	-	Print last computed wavefunction
PROJECTILE	off	Projectile B.S. definition is being input
QUADRATIC	on	Use parabolic extrapolation in B.S. search
QUAVER	off	Use the QUAVER quasi-Newton fitter
RADIALINT	off	Input is for radial integration stage
REINITIALIZ	0	Number of iterations between reinitialization of the fitter (mainly for POWELL65)
RENAME	-	Change the name of an object in the allocator
RESET	-	Initialize for a new calculation - allocator is CLEARed and all keywords set to initial stat
RETURN	-	Terminate Ptolemy
ROCORD	off	Use the ROCORD generalized minimizer
SAVEHS	off	Form factor integrals will be saved
SAVEWAVE	off	Scattering wavefunctions saved in allocator
SCATTERING	off	Input is for stand-alone scattering
SKIPASYMP	off	Do not use Whittaker function as asymptotic form of B.S. wavefunctions
TARGET	off	Input is for Target B.S.
TSO	none*	Operating in interactive mode - errors allow corrections and retries
UNDEFINE	-	Set a keyword to undefined status
USECOULOMB	on	Use Coulomb with core corrections in the interaction potential
USEHS	off	Use previously computed form factor integrals
USEPROJECTILE	on	Use projectile B.S. potential as the interaction potential
USESIMPCOUL	off	Use Coulomb of just one B.S. in the interaction potential

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* A value will be computed by the program if one is not given by the user.

Control and option-selecting keywords

Keyword	Default	Meaning
USETARGET	off	Use target B.S. potential as the interaction potential
WRITENS	-	Write an object onto Fortran file 15
WRITESTEP	none	Interval (fm) at which wavefunctions are to be tabulated

Sub-keywords for DATA

The following are keywords that may appear within the paraentheses that follow the DATA keyword.

Keyword	Default	Meaning
ANGLE	-	C.m. angles of the data are being entered
ANGLESHIFT	0	Amount (in degrees) bywhich the angles are to be shifted in the laboratory frame
ELAB	previous value	Laboratory energy of the data
MBERROR	-	Data errors are in millibarns
PERCENTERR	-	Data errors are in percent
RENORMALIZA	1	A quantity that will multiply each experimental cross section
SIGMA	-	Data is cross section in mb
SIGMATORUTH	-	Data is ratio of cross section to Rutherford cross section
WEIGHT	1	Each term in the chi-squared sum for the present data group is multiplied by WEIGHT

Appendix B - Core and CPU Time Estimates

Many Ptolemy calculations can be carried out in the Argonne Express class limits of 250K and 2 minutes. However large calculations may exceed one or both of these limits and in such cases it is useful to be able to estimate the core and time requirements of the job. One method of so doing is to compare the "Peak Compressed Size" line with the "Allocator Size" line in the "Allocator Statistics" that are printed at the end of each job. The difference of these two numbers is the amount by which the REGION specified on the JOB card may be reduced in future runs of similar calculations. The Peak Compressed Sizes from several jobs with varying L-ranges or grid sizes may also be used to estimate the needs of other calculations.

The more direct approach is to use the following formidable formulas to estimate the job requirements. New users of Ptolemy should not be frightened by these formulas; they should simply ignore the rest of this section until they are forced to consider it. In deriving these formulas an assumption was made about what part of the calculation would dominate in core and time requirements. Strange choices of grid parameters can violate this assumption in which case quite different results for the core and/or time requirements would occur. However for most Ptolemy runs the core estimate is quite accurate. The time estimate is not so good and can overestimate the required time by amounts up to 30%. Part of this overestimate is due to the inability to foresee how many integrands will be skipped because they are smaller than DWCUTOFF.

The core size that should be given in the REGION parameter on the JOB card is determined by the size of the Ptolemy program and associated I/O buffers and by the Peak Compressed Size of the allocator. The first size is at present 80K. The second size can be estimated from the following formulas:

1) Standard or SAVEHS Ptolemy run:

```
   Allocator(Kilobytes) = (1/128) * {
              NPSUM*NPDIF*( 2*NPPHI + Lxmax + 7/2 )
        + .5 * (Lxmax+Lxmin+2)(Lxmax-Lxmin+1) *
                 [ (Limax/2+1)(Lxmax+1)(Min{LbndP,LbndT}+1)
                   + 2(LMAX-LMIN+1)/LSTEP ]
        + (Limax+1)[ 17 + Max(Lxmax+LbndP, Lxmax+LbndT,
                              LbndP+LbndT+1) ]
        + 6*ASYMPTOPIA/STEPSIZE
        + 500 }
where
   Limax = LMAX + Lxmax
   LbndP = Projectile bound state L,
   LbndT = Target bound state L.
```

2) USEHS run:

Allocator(Kilobytes) = (1/128) * {
Max[NPSUM*NPDIF*(7/2 + Lxmax) + 8*(Limax+1)
+ 6*ASYMPTOPIA/STEPSIZE ,
(5+Lxmax)(Limax+1) + NumLiLoutLx' + NumAngles]
+ 6*(Limax+1)
+ NumLiLoutLx/LSTEP
+ 300 }

where

NumLiLoutLx = (LMAX-LMIN+1)(Lxmax+Lxmin+2)(Lxmax-Lxmin+1)
NumLiLoutLx' = (Lmax'-LMIN+1)(Lxmax+Lxmin+2)(Lxmax-Lxmin+1)
Lmax' = value of Li, Lout up to which extrapolation is performed
NumAngles = (ANGLEMAX-ANGLEMIN)/ANGLESTEP + 1

The time estimate for a standard or SAVEHS run on the 370/195 is given in the following formula. Timings on other computers will be approximately proportional to this estimate. No estimate is given for USEHS runs since they are so fast.

Time(seconds) = 10^{-7} * NPSUM*NPDIF*NPPHI *
[$(LMAX^2 - LMIN^2)$/LSTEP] *
(LbndP+1)(LbndT+1) *
{ 2 + (Lxmax+1)[Min(LbndP,LbndT)+1] }
+ (3 to 6)

As an example of the above formulas we consider the $^{208}Pb(^{16}O, ^{15}N)^{209}Bi(7/2^-)$ reaction for which

LbndP = 1 ,
LbndT = 3 ,
Lxmin = 3 ,
Lxmax = 4 .

The core estimate is

Core = (1/128) * { NPSUM*NPDIF*(2*NPPHI + 7.5)
+ 9*[5*LMAX + 30 + 2(LMAX-LMIN+1)/LSTEP]
+ 24*(LMAX+5)
+ 2*ASYMPTOPIA/STEPSIZE + 500 }

If we further assume

LMIN = 35 ,
LMAX = 70 ,
LSTEP = 5 ,
ASYMPTOPIA = 30 ,
STEPSIZE = .05 ,

we find

Core = NPSUM*NPDIF*(2*NPPHI+7.5)/128 + 56

which gives an estimate of 105K for NPSUM = 24, NPDIF = 10, NPPHI = 10 (the actual required size is 102K).

Similarly the time estimate for this case is

Time = NPSUM*NPDIF*NPPHI *
(LMAX**2-LMIN**2)/LSTEP * 10^{-5} ,
= NPSUM*NPDIF*NPPHI * 1.2*10^{-2} ,
= 17 seconds.

which is to be compared with the actual CPU time of 17 seconds.

Appendix C - JCL for Ptolemy Jobs at Argonne

Ptolemy runs that involve no KEEP, SAVEHS or USEHS commands may be made with the following JCL:

```
//jobname  JOB  (Fbadge,2,0,2),CLASS=C,REGION=250K
      account card
//   EXEC  PTOLEMY
      Ptolemy input
```

The above procedure defines FT06F001 as the output file, FT05F001 as the input, and STEPLIB as C109.PHYSICS.LOAD which contains the current production version of Ptolemy. For large calculations it may be necessary to modify the 2-minute time estimate or the 250K region estimate on the JOB card. The cost of small calculations can be slightly reduced by specifying a REGION of 200K or even 150K.

If a KEEP operation is to be made in a Ptolemy run, it is necessary to have a Speakeasy Keep dataset. This dataset must be a partitioned dataset with RECFM=FB, LRECL=80, and a reasonable block size such as BLKSIZE=1680. For ease in Speakeasy KEPT operations its name (at Argonne) should be Bnnnnn.SPEAKEZ.DATA where nnnnn is the user's badge number. Such a dataset is most easily made by logging on to TSO and using the ISPEAKEP command. Once the dataset has been made it will last indefinitely so one should not reuse the ISPEAKEP command for subsequent Ptolemy runs. Eventually the keep dataset will fill up so that from time to time it will be necessary to delete members and compress the dataset, or to make new keep datasets.

When one has a keep dataset, it may be used in Ptolemy runs with the following JCL:

```
//jobname  JOB  ... as above ...
      account card
//   EXEC  PTOLEMY
//MYKEEP   DD  DSN=Bnnnnn.SPEAKEZ.DATA,DISP=OLD
      Ptolemy input
```

The SAVEHS and USEHS commands use unformatted Fortran I/O. This requires a sequential dataset with the characteristics of RECFM=VBS,BLKSIZE=bbbb where bbbb is a reasonable size (3500 for 2314 drives or 4200 for 3330 drives). Ptolemy uses a special version of the Fortran I/O table that defaults to BLKSIZE=4200 so for 3330's it is not necessary to define BLKSIZE. Suitable JCL for a SAVEHS job is

```
//jobname  JOB  ... as above ...
     account card
//  EXEC  PTOLEMY
//FT01F001 DD DSN=C109.Bnnnnn.somename,DISP=(NEW,CATLG),
//    UNIT=SHRT3330,SPACE=(TRK,(19,19),RLSE),DCB=RECFM=VBS
     Ptolemy input
```

This JCL will make a dataset that lasts one week, if it is anticipated that the dataset will be used for a longer time, UNIT=LONG3330 should be used. In the later case the dataset should be deleted when one is done with it. If KEEP operations are to be done in the same job, then the MYKEEP DD card should also be included (either before or after the FT01F001 DD card).

USEHS runs may be made with the following JCL:

```
//jobname  JOB  ... as above ...
     account card
//  EXEC  PTOLEMY
//FT01F001 DD DSN=C109.Bnnnnn.somename,DISP=SHR
     Ptolemy input
```

Again the MYKEEP DD card should be included for KEEP operations.

Ptolemy may be used in TSO at Argonne by entering the command

```
EXEC 'B21541.PROC.CLIST(PTOLEMY)'
```

This command accesses an experimential version of Ptolemy that undergoes rather frequent changes and which will occasionally contain bugs. If one intends to do KEEP operations in the TSO session, one should invoke Ptolemy with the following two commands:

```
ALLOC F(MYKEEP) DA(SPEAKEZ.DATA)
EXEC 'B21541.PROC.CLIST(PTOLEMY)'
```

Appendix D - Sample Ptolemy Jobs

The following is the input for three sample Ptolemy jobs. These jobs use standard Ptolemy input sequences and, to reduce confusion, do not explore the alternative ways of defining a problem. The outputs of these examples are separately available from the authors of this report. The first sample shows a calculation with no KEEP or SAVEHS, USEHS keywords. In this case the orbital angular momenta of the bound states are not specified since Ptolemy can uniquely determine them.

```
//SPTOLEMY JOB (P88888,2,0,2),CLASS=C,REGION=200K
     PIEPER S    21541        56501-00109
//  EXEC  PTOLEMY
HEADER          TEST CASE   C
REACTION:  48CA(160 14C)50TI    ELAB = 56
PARAMETERSET CA60A
PROJECTILE
NODES = 1
R0 = 1.25  A = .65  V = 80    RC0 = 1.25
     ;
TARGET
NODES = 3
V = 100
     ;
INCOMING
V = 36.9  A = .4175  R0 = 1.35  RC0 = 1.2
VI = 78  RI0 = 1.27  AI = .28
;
OUTGOING
V = 36.9   VI = 78
;
;  $ This final semicolon starts the DWBA
KEYWORDS
RETURN
```

In the following example we have both SAVEHS and KEEP commands. Note that for the target state which has a spin orbit force, JP is not specified since it can be found from the other known spins.

```
//SPTOLEMY JOB (P88888,2,0,2),CLASS=C,REGION=250K
     PIEPER S    21541        56501-00109
//  EXEC  PTOLEMY
//MYKEEP    DD  DSN=B21541.SPEAKEZ.DATA,DISP=OLD
//FT01F001  DD  DSN=C109.PIEPER.PBBI7,DISP=(NEW,CATLG),
//  UNIT=SHRT3330,SPACE=(TRK,(19,19),RLSE),DCB=RECFM=VBS
HEADER:  EXAMPLE WITH BOTH  SAVEHS  AND  KEEP
REACTION:   208PB(160 15N)209BI(7/2- .90)  ELAB = 104
SAVEHS
PARAMETERSET PB100A
PROJECTILE
NODES = 0   L = 1
R0 = 1.20  A=.65  V=60  RC0 = 1.25 ;
TARGET
NODES = 1   L = 3
R0 = 1.28   A=.76   V=60
TAU = .099558  ;
INCOMING
V=40.   A=.45   R0 = 1.31  RC0 = 1.30
VI = 15
;
OUTGOING
V = 40   VI = 15
;
ANGLEMAX = 120  ;
KEEP CROSSSEC PBBI7A45
KEYWORDS
RETURN
```

The final DWBA example is a USEHS run that refers to the output of the previous example. The difference between the two calculations is that here A = .35 for the optical potentials. The ANGLEMAX card in this run is unnecessary since the value from the SAVEHS run would be used. However it can be used to produce a different angle grid from that used in the SAVEHS run. Note the small REGION size that may be used for USEHS's runs.

```
//SPTOLEMY JOB (P88888,2,0,2),CLASS=C,REGION=150K,MSGLEVEL=(0,0)
     PIEPER S    21541        56501-00109
//  EXEC  PTOLEMY
//MYKEEP    DD  DSN=B21541.SPEAKEZ.DATA,DISP=OLD
//FT01F001  DD  DSN=C109.PIEPER.PBBI7,DISP=SHR
HEADER:  EXAMPLE WITH BOTH  USEHS  AND  KEEP
USEHS
$  NOTE ABSENCE OF REACTION, GRID AND BOUND STATE
$  DEFINITIONS.
INCOMING
V=40.   A=.35   R0 = 1.31  RC0 = 1.30
VI = 15
;
OUTGOING
V = 40   VI = 15
;
ANGLEMAX = 120  ;
KEEP CROSSSEC PBBI7A35
KEYWORDS
RETURN
```

The following is an example of a five-parameter optical model fit to data at two energies. The depth of the real part of the potential is given an energy dependance while the rest of the potential parameters have no energy dependance. All of the potential radii will be equal to each other throughout the search while the real and imaginary diffusenesses will be separately varied. The search is first made with differential cross sections of moderate precision and is then repeated with more accurate values. Finally the differential cross sections for the two energies are printed on a uniform angular grid.

```
//SPTOL8 JOB (P88888,2,0,2),CLASS=C,REGION=150K,MSGLEVEL=(0,0)
 MACFARLANE M21541        56501-00109
//*
// EXEC PTOLEMY
CHANNEL:  160 + 208PB
HEADER:  EXAMPLE OF A TWO ENERGY FIT
FIT ( R0=RI0=RC0  A  AI  V VF )
R0 = 1.3    A = .5  AI = .5  V = 40, VE = -.2     VI = 15
DATA  (  ELAB=104  ANGLE  SIGMATORU  PERCENTER
$   KOVAR ET.AL.    O16 ON PB208 AT 104 MEV
26.87        1.120       15.
32.21        0.994       5.
37.54        1.005       5.
42.84        1.006       5.
45.49        1.010       5.
48.13        1.000       10.
50.76        1.017       5.
53.39        1.020       10.
56.01        1.083       5.
58.62        1.170       5.
61.23        1.200       5.
63.83        1.120       10.
66.43        0.991       5.
69.01        0.790       10.
71.59        0.599       5.
74.16        0.432       15.
76.72        0.290       10.
79.27        0.209       10.
84.36        0.086       15.
89.40        0.038       10.
$   KOVAR ET.AL. O16 ON PB208 AT  $    ELAB = 140    WEIGHT = .3
 10.8         0.932       5.0
 16.1         1.130       5.0
 21.5         1.050       2.0
 27.9         1.040       2.0
 32.2         0.975       2.0
 37.5         1.190       2.0
 42.8         0.877       2.0
 45.5         0.628       5.0
 48.1         0.286       5.0
 53.4         0.061       5.0
 58.6         0.014       5.0
```

```
      )
      ;
STEPSPER = 12   LMINMULT = .6   LMAXADD = 35   FITACCURACY = .0002
ELASTIC SCATTERING
ELAB = 104 ;
ELAB = 140 ;
RETURN
```